FILE 'HOME' ENTERED AT 08:29:47 ON 21 JUN 2009

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.22 0.22

FILE 'REGISTRY' ENTERED AT 08:30:00 ON 21 JUN 2009
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STRUCTURE FILE UPDATES: 19 JUN 2009 HIGHEST RN 1159249-84-9
DICTIONARY FILE UPDATES: 19 JUN 2009 HIGHEST RN 1159249-84-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when
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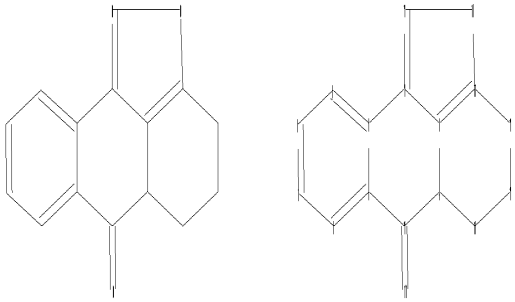
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10591974.str



chain nodes :
17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
10-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-15 8-9 8-11 9-10 9-14 11-12
11-16 12-13 13-14 15-16
exact/norm bonds :
4-7 5-10 7-8 7-15 8-9 8-11 9-10 9-14 10-17 11-12 11-16 12-13 13-14
15-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS

L1 STRUCTURE UPLOADED

=> s l1 sss sam
SAMPLE SEARCH INITIATED 08:30:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 495 TO ITERATE

100.0% PROCESSED 495 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8566 TO 11234
PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 08:30:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9220 TO ITERATE

100.0% PROCESSED 9220 ITERATIONS 59 ANSWERS
SEARCH TIME: 00.00.01

L3 59 SEA SSS FUL L1

=> file capl
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 186.10

FILE 'CAPLUS' ENTERED AT 08:30:28 ON 21 JUN 2009
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FILE COVERS 1907 - 21 Jun 2009 VOL 150 ISS 26
FILE LAST UPDATED: 19 Jun 2009 (20090619/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 21 L3

=> help roles

CAS roles are CAS indexing terms consisting of codes that describe the new or novel information reported about a substance or a class of compounds. Specific roles have 3-letter codes. Super roles have 4-letter codes. Super roles are automatically generated from the specific roles, and are upposted for searching.

To search a role for a specific substance, append the CAS Registry Number or a Registry File L-number answer set with a slash and the code for the role, e.g., 67-68-5/THU. To search more than one role, separate a list of roles by commas and no spaces, e.g., 67-68-5/THU,ADV. Only one role may be appended to an L-number answer set. Use the OR operator to apply multiple roles to an L-number, e.g., S L1/THU OR L1/ADV.

To search roles assigned to index headings for classes of compounds, follow the heading with a slash and the role or roles separated by commas, e.g., PHENOLS/POL,REM.

Roles are displayed in the RL (Role) field within the IT (Index Term) field. Roles are included in any display format that contains the IT or RL field. Enter SET ROLES OFF at an arrow prompt (=>) to suppress display of codes and text for roles. Enter SET ROLES CODES to display only codes. Enter SET ROLES TEXT to return to default display (codes and names). Enter HELP SET ROLES at an arrow prompt for more information.

Enter HELP THESAURUS and HELP RCODE at an arrow prompt in this file for information on using the role thesaurus to find role definitions and narrower and broader terms.

In the following list, under each super role are listed the specific roles that generate the super role.

List of CAS Roles (1)

ANST Analytical Study

ANT Analyte
AMX Analytical Matrix
ARG Analytical Reagent Use
ARU Analytical Role, Unclassified

BIOL Biological Study

ADV Adverse Effect, Including Toxicity
AGR Agricultural Use
BAC Biological Activity or Effector, Except Adverse (2)
BCP Biochemical Process (3)
BMF Bioindustrial Manufacture
BOC Biological Occurrence (2)
BPN Biosynthetic Preparation
BPR Biological Process (2)
BSU Biological Study, Unclassified
BUU Biological Use, Unclassified
COS Cosmetic Use (3)
DGN Diagnostic Use (3)
DMA Drug Mechanism of Action (3)
FFD Food or Feed Use
MFM Metabolic Formation (2)
NPO Natural Product Occurrence (3)
PAC Pharmacological Activity (3)
PKT Pharmacokinetics (3)
THU Therapeutic Use

CMBI Combinatorial Study (3)

CPN Combinatorial Preparation (3)
CRT Combinatorial Reactant (3)
CRG Combinatorial Reagent (3)
CST Combinatorial Study (3)
CUS Combinatorial Use (3)

FORM Formation, Nonpreparative

FMU Formation, Unclassified
GFM Geological or Astronomical Formation
MFM Metabolic Formation (2)

NANO Nanomaterial (4)

OCCU Occurrence

BOC Biological Occurrence (2)
GOC Geological or Astronomical Occurrence
NPO Natural Product Occurrence (3)
OCU Occurrence, Unclassified
POL Pollutant

PREP Preparation (5)

BMF Bioindustrial Manufacture
BPN Biosynthetic Preparation
BYP Byproduct
CPN Combinatorial Preparation (3)
IMF Industrial Manufacture
PUR Purification or Recovery
PNU Preparation, Unclassified (6)
SPN Synthetic Preparation

PROC Process

BCP Biochemical Process (3)

BPR Biological Process (2)
GPR Geological or Astronomical Process
PEP Physical, Engineering, or Chemical Process
CPS Chemical Process (7)
EPR Engineering Process (7)
PYP Physical Process (7)
REM Removal or Disposal

PRPH Prophetic Substance (8)

RACT Reactant or Reagent (2,7)

RCT Reactant (9)
 CRT Combinatorial Reactant (3)
RGT Reagent (3)
 CRG Combinatorial Reagent (3)

USES Uses

AGR Agricultural Use
ARG Analytical Reagent Use
BUU Biological Use, Unclassified
CAT Catalyst Use
COS Cosmetic Use (3)
CUS Combinatorial Use (3)
DGN Diagnostic Use (3)
FFD Food or Feed Use
MOA Modifier or Additive Use
NUU Other Use, Unclassified (10)
POF Polymer in Formulation
TEM Technical or Engineered Material Use
THU Therapeutic Use

Specific roles that are not upposted to any super roles:

MSC Miscellaneous
PRP Properties

(1) Super roles have 4-letter codes. Specific roles have 3-letter codes. Under each super role are listed the corresponding specific roles that are retrieved when you search that super role.
(2) Used from CA Vol. 66 (1967) to Vol. 135 (2001)
(3) Used starting with CA Vol. 136 (2002)
(4) Used starting with records in 1992.
(5) The PREP super role has been added to records back to 1907.
(6) Used from CA vol. 66 (1967) to vol. 145 (2006).
(7) Used from CA vol. 136 (2002) to CA vol. 145 (2006).
(8) Used starting with records from 2003.
(9) Searching the RCT (Reactant) role retrieves references from CA Vol. 66 (1967) to the present. Searching the RACT (Reactant or Reagent) super role retrieves references with the CRT, CRG, RGT, or RCT references starting with CA Vol. 136 (2002).
(10) Starting with CA Vol. 136 (2002), the searchable text for the NUU role changed from NONBIOLOGICAL USE, UNCLASSIFIED/RL to OTHER USE, UNCLASSIFIED/RL. Search the code NUU/RL to retrieve records from CA Vol. 66 (1967) to the present.

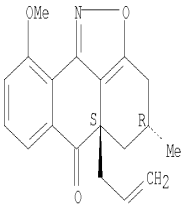
=> s l4 and (prep/rl OR spn/rl)

      4797148 PREP/RL
      2218397 SPN/RL
L5   10 L4 AND (PREP/RL OR SPN/RL)

=> d 1-10 ibib hitstr

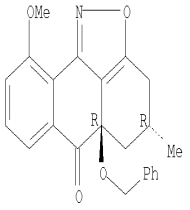
L5 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:11627 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 150:237267
TITLE: Isoxazole-assisted direct substitution of the hydroxy group in α-ketols: Introduction of angular substituents in a polycyclic system
AUTHOR(S): Takikawa, Hiroshi; Hikita, Katsuyoshi; Suzuki, Keisuke
CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology, SORST-JST Agency, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2008), 47(51), 9887-9890
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 1116151-26-8P 1116151-29-1P 1116151-30-4P
    1116151-31-5P 1116151-32-6P
    RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
      (crystal structure; introduction of angular substituents in a polycyclic system via isoxazole-assisted direct substitution of the hydroxy group in α-ketols)
RN 1116151-26-8 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-10-methoxy-4-methyl-5a-(2-propen-1-yl)-, (4R,5aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



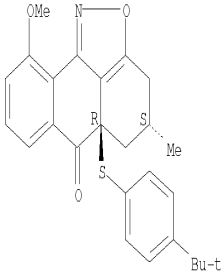
RN 1116151-29-1 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-10-methoxy-4-methyl-5a-(phenylmethoxy)-, (4R,5aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



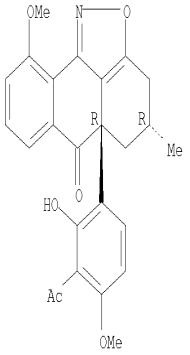
RN 1116151-30-4 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-[[4-(1,1-dimethylethyl)phenyl]thio]-3,4,5,5a-tetrahydro-10-methoxy-4-methyl-, (4R,5aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



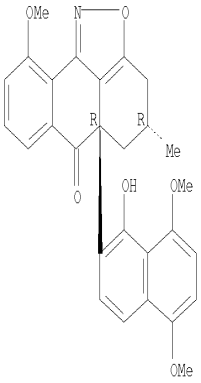
RN 1116151-31-5 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-(3-acetyl-2-hydroxy-4-methoxyphenyl)-3,4,5,5a-tetrahydro-10-methoxy-4-methyl-, (4R,5aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



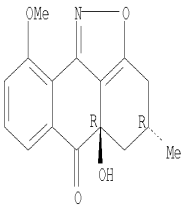
RN 1116151-32-6 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(1-hydroxy-5,8-dimethoxy-2-naphthalenyl)-10-methoxy-4-methyl-, (4R,5aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



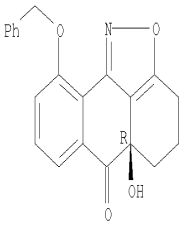
IT 577975-48-5 943151-35-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(introduction of angular substituents in a polycyclic system via isoxazole-assisted direct substitution of the hydroxy group in α-ketols)
RN 577975-48-5 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-methoxy-4-methyl-, (4R,5aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



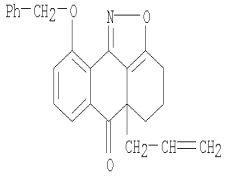
RN 943151-35-7 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(phenylmethoxy)-, (5aR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



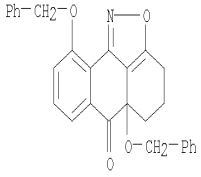
IT 943151-62-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(introduction of angular substituents in a polycyclic system via isoxazole-assisted direct substitution of the hydroxy group in α-ketols)

RN 943151-62-0 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-10-(phenylmethoxy)-5a-(2-propen-1-yl)- (CA INDEX NAME)

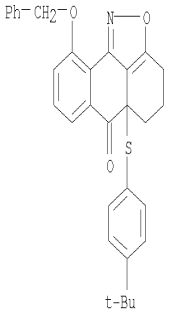


IT 1116151-09-7P 1116151-10-0P 1116151-12-2P
1116151-13-3P 1116151-14-4P 1116151-15-5P
1116151-18-8P 1116151-19-9P 1116151-20-2P
1116151-21-3P 1116151-23-5P 1116151-24-6P
1116151-25-7P 1116151-28-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(introduction of angular substituents in a polycyclic system via isoxazole-assisted direct substitution of the hydroxy group in α-ketols)

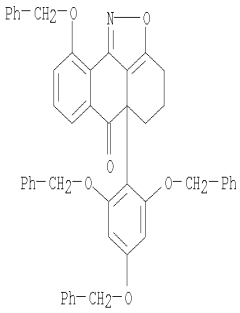
RN 1116151-09-7 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a,10-bis(phenylmethoxy)- (CA INDEX NAME)



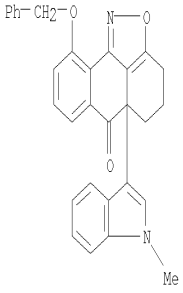
RN 1116151-10-0 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-[[4-(1,1-dimethylethyl)phenyl]thio]-3,4,5,5a-tetrahydro-10-(phenylmethoxy)- (CA INDEX NAME)



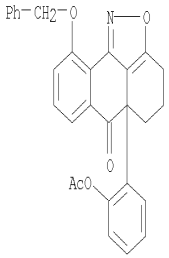
RN 1116151-12-2 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-10-(phenylmethoxy)-5a-[2,4,6-tris(phenylmethoxy)phenyl]- (CA INDEX NAME)



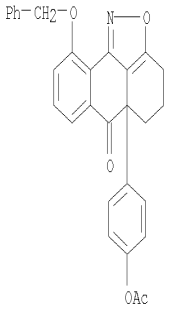
RN 1116151-13-3 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(1-methyl-1H-indol-3-yl)-10-(phenylmethoxy)- (CA INDEX NAME)



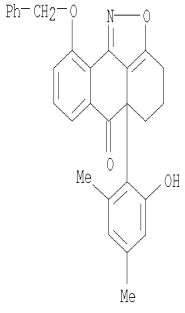
RN 1116151-14-4 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-[2-(acetyloxy)phenyl]-3,4,5,5a-tetrahydro-10-(phenylmethoxy)- (CA INDEX NAME)



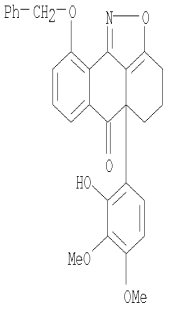
RN 1116151-15-5 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-[4-(acetyloxy)phenyl]-3,4,5,5a-tetrahydro-10-(phenylmethoxy)- (CA INDEX NAME)



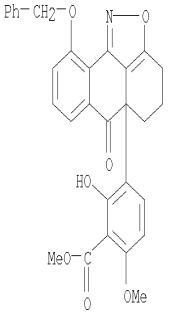
RN 1116151-18-8 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(2-hydroxy-4,6-dimethylphenyl)-10-(phenylmethoxy)- (CA INDEX NAME)



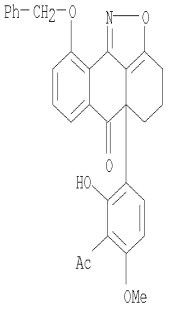
RN 1116151-19-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(2-hydroxy-3,4-dimethoxyphenyl)-10-(phenylmethoxy)- (CA INDEX NAME)



RN 1116151-20-2 CAPLUS
CN Benzoic acid, 3-[4,5-dihydro-6-oxo-10-(phenylmethoxy)-3H-anthra[9,1-cd]isoxazol-5a(6H)-yl]-2-hydroxy-6-methoxy-, methyl ester (CA INDEX NAME)

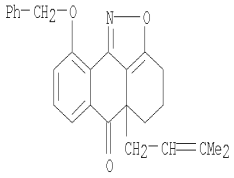


RN 1116151-21-3 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-(3-acetyl-2-hydroxy-4-methoxyphenyl)-3,4,5,5a-tetrahydro-10-(phenylmethoxy)- (CA INDEX NAME)

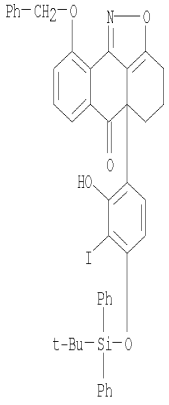


RN 1116151-23-5 CAPLUS

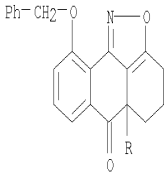
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(3-methyl-2-buten-1-yl)-10-(phenylmethoxy)- (CA INDEX NAME)

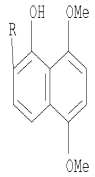


RN 1116151-24-6 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-[4-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-hydroxy-3-iodophenyl]-3,4,5,5a-tetrahydro-10-(phenylmethoxy)- (CA INDEX NAME)



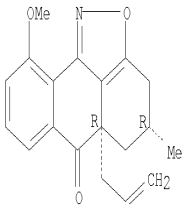
RN 1116151-25-7 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(1-hydroxy-5,8-dimethoxy-2-naphthalenyl)-10-(phenylmethoxy)- (CA INDEX NAME)





RN 1116151-28-0 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-10-methoxy-4-methyl-5a-(2-propen-1-yl)-, (4R,5aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



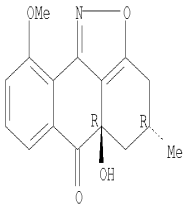
REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1200735 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 149:576027
TITLE: Formation of α-hydroxy-β-diketones through hydroxylation of isoxazolium salts: stereoselective approach to angular cis-diols in polycyclic systems
AUTHOR(S): Takikawa, Hiroshi; Takada, Akiomi; Hikita, Katsuyoshi; Suzuki, Keisuke
CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology, SORST-JST Agency, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2008), 47(39), 7446-7449
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:576027
IT 577975-48-5 577975-49-6 943151-35-7

1084894-65-4 1084894-67-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of α-hydroxy-β-diketones through N-methylation of isoxazoles with trimethyloxonium tetrafluoroborate and hydroxylation of isoxazolium salts)

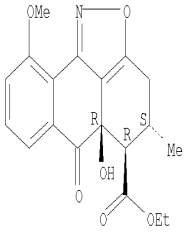
RN 577975-48-5 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-methoxy-4-methyl-, (4R,5aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



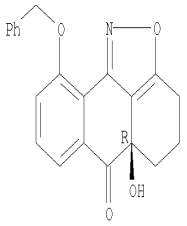
RN 577975-49-6 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5-carboxylic acid, 4,5,5a,6-tetrahydro-5a-hydroxy-10-methoxy-4-methyl-6-oxo-, ethyl ester, (4R,5S,5aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

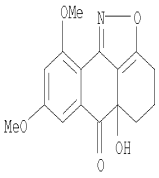


RN 943151-35-7 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(phenylmethoxy)-, (5aR)- (CA INDEX NAME)

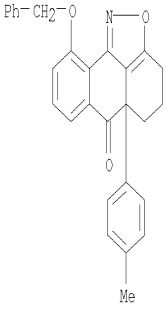
Absolute stereochemistry. Rotation (+).



RN 1084894-65-4 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-8,10-dimethoxy- (CA INDEX NAME)



RN 1084894-67-6 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(4-methylphenyl)-10-(phenylmethoxy)- (CA INDEX NAME)



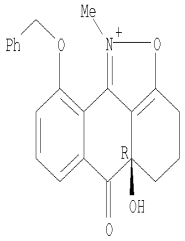
IT 1084894-59-6P 1084894-69-8P 1084894-71-2P
1084894-73-4P 1084894-78-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of α-hydroxy-β-diketones through N-methylation of isoxazoles with trimethyloxonium tetrafluoroborate and hydroxylation of isoxazolium salts)

RN 1084894-59-6 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazolium, 4,5,5a,6-tetrahydro-5a-hydroxy-1-methyl-6-oxo-10-(phenylmethoxy)-, (5aR)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

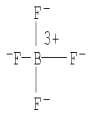
CRN 1084894-58-5
CMF C22 H20 N O4

Absolute stereochemistry.



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

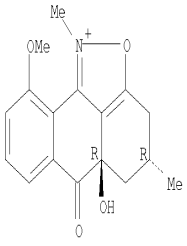


RN 1084894-69-8 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazolium, 4,5,5a,6-tetrahydro-5a-hydroxy-1,4-dimethyl-6-oxo-10-methoxy-, (4R,5aR)-rel-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

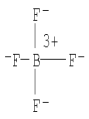
CRN 1084894-68-7
CMF C17 H18 N O4

Relative stereochemistry.



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

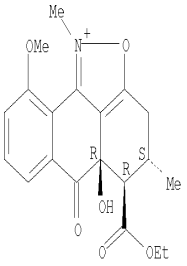


RN 1084894-71-2 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazolium, 5-(ethoxycarbonyl)-4,5,5a,6-tetrahydro-5a-hydroxy-10-methoxy-1,4-dimethyl-6-oxo-, (4R,5S,5aS)-rel-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

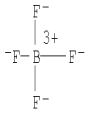
CRN 1084894-70-1
CMF C20 H22 N O6

Relative stereochemistry.



CM 2

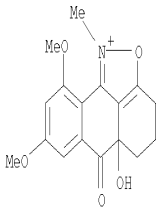
CRN 14874-70-5
CMF B F4
CCI CCS



RN 1084894-73-4 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazolium, 4,5,5a,6-tetrahydro-5a-hydroxy-8,10-dimethoxy-1-methyl-6-oxo-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

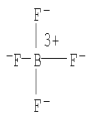
CM 1

CRN 1084894-72-3
CMF C17 H18 N O5



CM 2

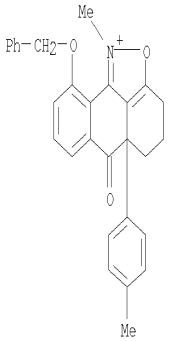
CRN 14874-70-5
CMF B F4
CCI CCS



RN 1084894-78-9 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazolium, 4,5,5a,6-tetrahydro-1-methyl-5a-(4-methylphenyl)-6-oxo-10-(phenylmethoxy)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

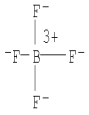
CM 1

CRN 1084894-77-8
CMF C29 H26 N O3



CM 2

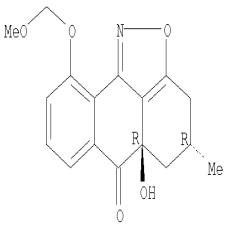
CRN 14874-70-5
CMF B F4
CCI CCS



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:190171 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 148:449823
TITLE: Total synthesis and structure assignment of the anthrone C-glycoside cassialoin
AUTHOR(S): Koyama, Yasuhito; Yamaguchi, Ryo; Suzuki, Keisuke
CORPORATE SOURCE: Department of Chemistry, SORST-JST Agency, Tokyo Institute of Technology, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2008), 47(6), 1084-1087
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:449823
IT 1017858-89-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and structure assignment of the anthrone C-glycoside cassialoin via isoxazole-containing stereogenic α-ketol and a subsequent intramol. redox reaction)
RN 1017858-89-7 CAPLUS
CN 6H-Athra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(methoxymethoxy)-4-methyl-, (4R,5aR)-rel- (CA INDEX NAME)

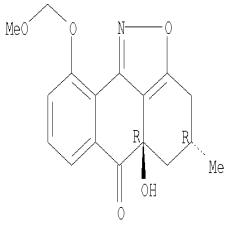
Relative stereochemistry.



IT 1017857-95-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and structure assignment of the anthrone C-glycoside cassialoin via isoxazole-containing stereogenic α-ketol and a subsequent intramol. redox reaction)

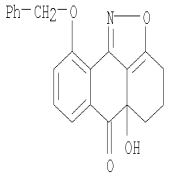
RN 1017857-95-2 CAPLUS
CN 6H-Athra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(methoxymethoxy)-4-methyl-, (4R,5aR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

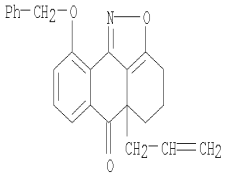


REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:546202 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 147:117809
TITLE: Isoxazole-directed pinacol rearrangement: stereocontrolled approach to angular stereogenic centers
AUTHOR(S): Suzuki, Keisuke; Takikawa, Hiroshi; Hachisu, Yoshifumi; Bode, Jeffrey W.
CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology, SORST-JST Agency, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2007), 46(18), 3252-3254
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:117809
IT 943151-61-9P 943151-62-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(racemates; stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)
RN 943151-61-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(phenylmethoxy)- (CA INDEX NAME)

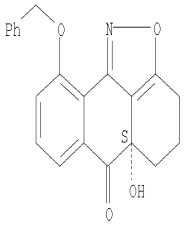


RN 943151-62-0 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-10-(phenylmethoxy)-5a-(2-propen-1-yl)- (CA INDEX NAME)



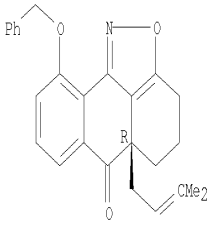
IT 943151-47-1P 943151-59-5P 943151-60-8P
943151-63-1P
RL: BYP (Byproduct); PREP (Preparation)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)
RN 943151-47-1 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(phenylmethoxy)-, (5aS)- (CA INDEX NAME)

Absolute stereochemistry.



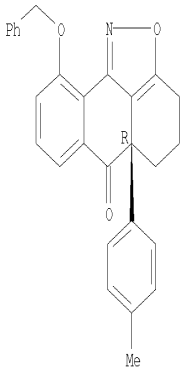
RN 943151-59-5 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(3-methyl-2-buten-1-yl)-10-(phenylmethoxy)-, (5aR)- (CA INDEX NAME)

Absolute stereochemistry.



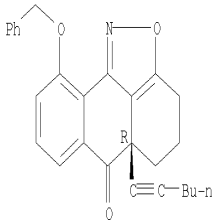
RN 943151-60-8 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(4-methylphenyl)-10-(phenylmethoxy)-, (5aR)- (CA INDEX NAME)

Absolute stereochemistry.



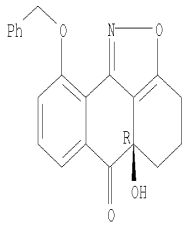
RN 943151-63-1 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-(1-hexyn-1-yl)-3,4,5,5a-tetrahydro-10-(phenylmethoxy)-, (5aR)- (CA INDEX NAME)

Absolute stereochemistry.



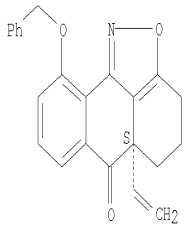
IT 943151-35-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)
RN 943151-35-7 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(phenylmethoxy)-, (5aR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



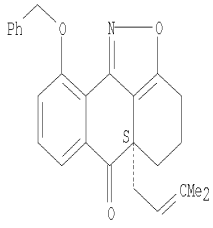
IT 943151-37-9P 943151-40-4P 943151-53-9P
943151-54-0P 943151-55-1P 943151-56-2P
943151-57-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)
RN 943151-37-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-ethenyl-3,4,5,5a-tetrahydro-10-(phenylmethoxy)-, (5aS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



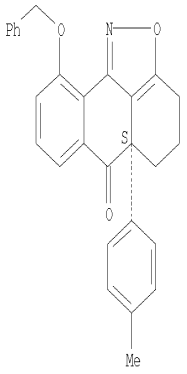
RN 943151-40-4 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(3-methyl-2-buten-1-yl)-10-(phenylmethyl)-, (5aS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



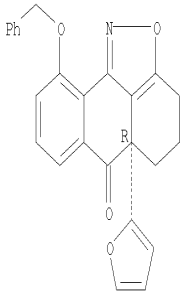
RN 943151-53-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(4-methylphenyl)-10-(phenylmethoxy)-, (5aS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



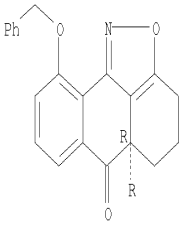
RN 943151-54-0 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-(2-furanyl)-3,4,5,5a-tetrahydro-10-(phenylmethoxy)-, (5aR)- (CA INDEX NAME)

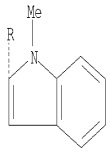
Absolute stereochemistry. Rotation (-).



RN 943151-55-1 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-(1-methyl-1H-indol-2-yl)-10-(phenylmethoxy)-, (5aR)- (CA INDEX NAME)

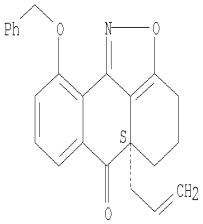
Absolute stereochemistry. Rotation (-).





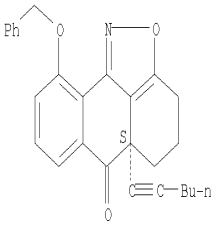
RN 943151-56-2 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-10-(phenylmethoxy)-5a-(2-propen-1-yl)-, (5aS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 943151-57-3 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 5a-(1-hexyn-1-yl)-3,4,5,5a-tetrahydro-10-(phenylmethoxy)-, (5aS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

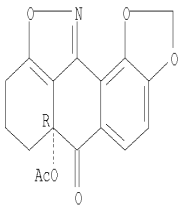


REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

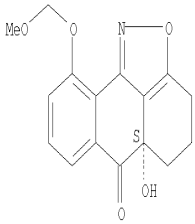
L5 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:546035 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 145:188145
TITLE: Catalytic enantioselective crossed aldehyde-ketone benzoin cyclization
AUTHOR(S): Takikawa, Hiroshi; Hachisu, Yoshifumi; Bode, Jeffrey W.; Suzuki, Keisuke
CORPORATE SOURCE: Department of Chemistry Tokyo Institute of Technology, SORST-JST Agency, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2006), 45(21), 3492-3494
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:188145
IT 901764-20-3P 902129-39-9P 902129-40-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of cyclic α-hydroxy ketones via triazolium salt-catalyzed enantioselective crossed aldehyde-ketone benzoin cyclization of ketoaldehydes)
RN 901764-20-3 CAPLUS
CN 6H-[1,3]Dioxolo[7,8]anthra[9,1-cd]isoxazol-6-one, 5a-(acetyloxy)-3,4,5,5a-tetrahydro-, (5aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



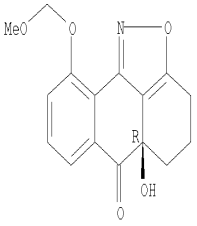
RN 902129-39-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(methoxymethoxy)-, (5aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 902129-40-2 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(methoxymethoxy)-, (5aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1023428 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 143:306299
TITLE: Preparation of polycyclic ketones having anthraisoxazole structure by pinacol rearrangement of diols
INVENTOR(S): Suzuki, Keisuke
PATENT ASSIGNEE(S): Japan Science and Technology Agency, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

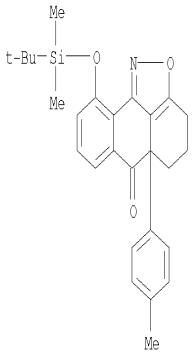
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005255592	A	20050922	JP 2004-67741	20040310
JP 4219289	B2	20090204		
WO 2005095422	A1	20051013	WO 2005-JP4723	20050310
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1724274	A1	20061122	EP 2005-720958	20050310
R: DE, FR, GB				
US 20070149786	A1	20070628	US 2006-591974	20060908

PRIORITY APPLN. INFO.: JP 2004-67741 A 20040310
WO 2005-JP4723 W 20050310
OTHER SOURCE(S): CASREACT 143:306299; MARPAT 143:306299
IT 864951-75-7P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation);

PREP (Preparation)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

RN 864951-75-7 CAPLUS

CN 6H-Anthra[9,1-cd]isoxazol-6-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3,4,5,5a-tetrahydro-5a-(4-methylphenyl)-(9CI) (CA INDEX NAME)

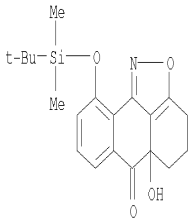


IT 864951-73-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

RN 864951-73-5 CAPLUS

CN 6H-Anthra[9,1-cd]isoxazol-6-one, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3,4,5,5a-tetrahydro-5a-hydroxy- (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004724 CAPLUS <<LOGINID::20090621>>

DOCUMENT NUMBER: 143:306298

TITLE: Preparation of polycyclic anthraquinone compounds by stereoselective intramolecular benzoin condensation

INVENTOR(S): Suzuki, Keisuke

PATENT ASSIGNEE(S): Japan Science and Technology Agency, Japan

SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085217	A1	20050915	WO 2005-JP4709	20050310
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005255594	A	20050922	JP 2004-67768	20040310
JP 4253603	B2	20090415		

PRIORITY APPLN. INFO.: JP 2004-67768 A 20040310

OTHER SOURCE(S): CASREACT 143:306298; MARPAT 143:306298

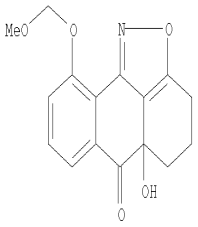
IT 864817-42-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of anthraisoxazolone via chiral triazolium-catalyzed enantioselective intramol. benzoin condensation of oxobenzisoxazolyl benzaldehyde in the presence of DBU)

RN 864817-42-5 CAPLUS

CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(methoxymethoxy)-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:411577 CAPLUS <<LOGINID::20090621>>

DOCUMENT NUMBER: 140:391270

TITLE: Preparation of isoxazole ring-containing polycyclic compounds as intermediates for anthraquinones

INVENTOR(S): Suzuki, Keisuke; Bode, Jeffrey W.

PATENT ASSIGNEE(S): Japan Science and Technology Agency, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF

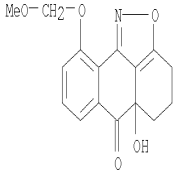
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

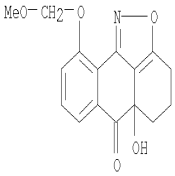
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004143082	A	20040520	JP 2002-309814	20021024
JP 4252788	B2	20090408		

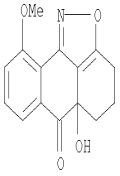
PRIORITY APPLN. INFO.: JP 2002-309814 20021024
OTHER SOURCE(S): CASREACT 140:391270; MARPAT 140:391270
IT 577975-39-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoxazole ring-containing polycyclic compds. as intermediates
for anthraquinones)
RN 577975-39-4 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(methoxymethoxy)- (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:473424 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 139:180004
TITLE: Catalytic Intramolecular Crossed Aldehyde-Ketone Benzoin Reactions: A Novel Synthesis of Functionalized Preanthraquinones
AUTHOR(S): Hachisu, Yoshifumi; Bode, Jeffrey W.; Suzuki, Keisuke
CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology and CREST, Japan Science and Technology Corporation, Tokyo, 152-8551, Japan
SOURCE: Journal of the American Chemical Society (2003), 125(28), 8432-8433
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:180004
IT 577975-39-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of anthracenone- or naphthalenone-fused isoxazoles via intramol. aldehyde-ketone benzoin condensation of (oxoalkyl)isoxazolyl benzaldehydes)
RN 577975-39-4 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-(methoxymethoxy)- (9CI) (CA INDEX NAME)

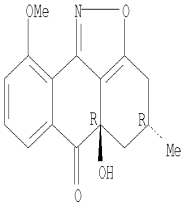


IT 577975-47-4P 577975-48-5P 577975-49-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of anthracenone- or naphthalenone-fused isoxazoles via intramol. aldehyde-ketone benzoin condensation of (oxoalkyl)isoxazolyl benzaldehydes)
RN 577975-47-4 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-methoxy- (9CI) (CA INDEX NAME)



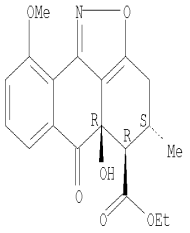
RN 577975-48-5 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 3,4,5,5a-tetrahydro-5a-hydroxy-10-methoxy-4-methyl-, (4R,5aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 577975-49-6 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5-carboxylic acid, 4,5,5a,6-tetrahydro-5a-hydroxy-10-methoxy-4-methyl-6-oxo-, ethyl ester, (4R,5S,5aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



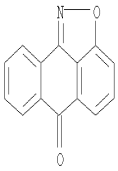
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:658099 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 137:201301
TITLE: Preparation of isothiazoloanthrones, isoxazoloanthrones, isoindolanthrones as JNK inhibitors
INVENTOR(S): Sakata, Steven T.; Raymon, Heather K.
PATENT ASSIGNEE(S): Signal Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 196 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

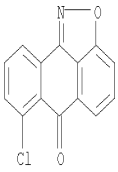
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002066450	A2	20020829	WO 2002-US4283	20020213
WO 2002066450	A3	20021205		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20030073732	A1	20030417	US 2002-71390	20020207
US 6987184	B2	20060117		
CA 2438312	A1	20020829	CA 2002-2438312	20020213
AU 2002251936	A1	20020904	AU 2002-251936	20020213
EP 1363891	A2	20031126	EP 2002-720975	20020213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004526711	T	20040902	JP 2002-565966	20020213
NZ 528034	A	20051223	NZ 2002-528034	20020213
US 20060004080	A1	20060105	US 2005-159592	20050622
US 7354947	B2	20080408		

PRIORITY APPLN. INFO.:	US 2001-269013P	P	20010215
	US 2002-71390	A	20020207
	WO 2002-US4283	W	20020213

OTHER SOURCE(S): MARPAT 137:201301
IT 63973-07-9P, 6H-Anthra[9,1-cd]isoxazol-6-one 452343-54-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isothiazoloanthrones, isoxazoloanthrones, isoindolanthrones as JNK inhibitors)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



RN 452343-54-3 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one, 7-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l4 not l5
L6 11 L4 NOT L5

=> d 1-11 ibib hitstr

L6 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1038135 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 145:389396
TITLE: JNK2 inhibition- and MAPK9 gene expression inhibition-based methods for treatment of type 1 diabetes
INVENTOR(S): Davis, Roger J.; Jaeschke, Anja
PATENT ASSIGNEE(S): University of Massachusetts Medical School, a Massachusetts Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 70pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060223807	A1	20061005	US 2005-92099	20050329
WO 2006104983	A1	20061005	WO 2006-US11038	20060328

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

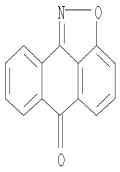
PRIORITY APPLN. INFO.: US 2005-92099 A 20050329

OTHER SOURCE(S): MARPAT 145:389396

IT 63973-07-9, 6H-Anthra[9,1-cd]isoxazol-6-one 63973-07-9D, 6H-Anthra[9,1-cd]isoxazol-6-one, derivs.
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(JNK2 inhibition-based methods for treatment of type 1 diabetes)

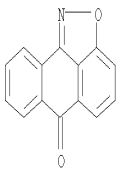
RN 63973-07-9 CAPLUS

CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



RN 63973-07-9 CAPLUS

CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



L6 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:513446 CAPLUS <<LOGINID::20090621>>

DOCUMENT NUMBER: 145:1054

TITLE: Methods and compositions using JNK inhibitors for treatment and management of central nervous system injury

INVENTOR(S): Zeldis, Jerome B.; Faleck, Herbert; Manning, Donald

PATENT ASSIGNEE(S): Celgene Corporation, USA

SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006058007	A2	20060601	WO 2005-US42330	20051118
WO 2006058007	A3	20060810		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

AU 2005309732	A1	20060601	AU 2005-309732	20051118
CA 2588558	A1	20060601	CA 2005-2588558	20051118
EP 1827422	A2	20070905	EP 2005-852021	20051118

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU

CN 101102767	A	20080109	CN 2005-80047030	20051118
JP 2008520730	T	20080619	JP 2007-543401	20051118
ZA 2007004889	A	20080925	ZA 2007-4889	20051118
US 20060122179	A1	20060608	US 2005-286128	20051122
MX 2007006066	A	20070711	MX 2007-6066	20070521
KR 2007086600	A	20070827	KR 2007-714354	20070622

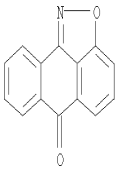
PRIORITY APPLN. INFO.: US 2004-630598P P 20041123
WO 2005-US42330 W 20051118

OTHER SOURCE(S): MARPAT 145:1054

IT 63973-07-9, 6H-Anthra[9,1-cd]isoxazol-6-one
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(JNK inhibitors for treatment of central nervous system injury)

RN 63973-07-9 CAPLUS

CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1259534 CAPLUS <<LOGINID::20090621>>

DOCUMENT NUMBER: 144:19239

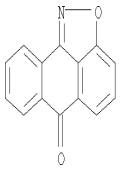
TITLE: Methods for preserving tissues during transplantation using JNK inhibitors

INVENTOR(S): Bennett, Brydon L.; Brenner, David A.; Zeldis, Jerome B.

PATENT ASSIGNEE(S): Celgene Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 27 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050266391	A1	20051201	US 2005-35842	20050114
PRIORITY APPLN. INFO.:			US 2004-537353P P	20040115

OTHER SOURCE(S): MARPAT 144:19239
IT 63973-07-9D, 6H-Anthra[9,1-cd]isoxazol-6-one, derivs.
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for preserving tissues during transplantation using JNK inhibitors)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



L6 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:451122 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 142:476230
TITLE: Methods of using and compositions comprising a JNK inhibitor for the treatment and management of asbestos-related diseases and disorders
INVENTOR(S): Zeldis, Jerome B.
PATENT ASSIGNEE(S): Celgene Corporation, USA
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005046594	A2	20050526	WO 2004-US37084	20041104
WO 2005046594	A3	20050922		

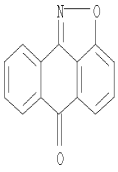
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004288715	A1	20050526	AU 2004-288715	20041104
CA 2544591	A1	20050526	CA 2004-2544591	20041104
EP 1684690	A2	20060802	EP 2004-800843	20041104

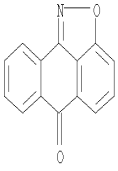
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR, IS, YU

BR 2004016266	A	20070109	BR 2004-16266	20041104
CN 1901903	A	20070124	CN 2004-80040002	20041104
JP 2007510671	T	20070426	JP 2006-538531	20041104
ZA 2006003719	A	20070926	ZA 2006-3719	20041104
MX 2006004997	A	20060714	MX 2006-4997	20060504
KR 2006124610	A	20061205	KR 2006-711021	20060605
US 20070270448	A1	20071122	US 2007-578809	20070312
PRIORITY APPLN. INFO.:			US 2003-518601P P	20031106
			WO 2004-US37084 W	20041104

OTHER SOURCE(S): MARPAT 142:476230
IT 63973-07-9, 6H-Anthra[9,1-cd]isoxazol-6-one 63973-07-9D, 6H-Anthra[9,1-cd]isoxazol-6-one, salts, monosubstituted, disubstituted
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(as JNK inhibitor; JNK inhibitor and compns. for treatment and management of asbestos-related diseases and disorders)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

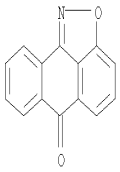
L6 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:589385 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 141:128915
TITLE: Drug-coated stents and methods of use therefor
INVENTOR(S): Zeldis, Jerome B.
PATENT ASSIGNEE(S): Celgene Corporation, USA

SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004060318	A2	20040722	WO 2003-US41763	20031231
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
ZA 2005005307	A	20060927	ZA 2005-5307	20021231
US 20050019366	A1	20050127	US 2003-749344	20031230
CA 2512056	A1	20040722	CA 2003-2512056	20031231
AU 2003300466	A1	20040729	AU 2003-300466	20031231
EP 1587440	A2	20051026	EP 2003-815013	20031231
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017909	A	20051129	BR 2003-17909	20031231
CN 1756531	A	20060405	CN 2003-80110071	20031231
JP 2006512143	T	20060413	JP 2004-564931	20031231
MX 2005006999	A	20050818	MX 2005-6999	20050627

PRIORITY APPLN. INFO.:
US 2002-437332P P 20021231
US 2003-749344 A 20031230
WO 2003-US41763 W 20031231

OTHER SOURCE(S): MARPAT 141:128915
IT 63973-07-9, 6H-Anthra[9,1-cd]isoxazol-6-one
RL: DEV (Device component use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(stents comprising JNK kinase inhibitor for treating or preventing cardiovascular or renal disease)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



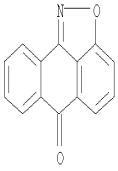
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:392328 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 140:386068
TITLE: Methods using a JNK inhibitor for the treatment, prevention and management of macular degeneration
INVENTOR(S): Zeldis, Jerome B.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 31 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040092568	A1	20040513	US 2003-699105	20031030
CA 2504028	A1	20040521	CA 2003-2504028	20031031
WO 2004041191	A2	20040521	WO 2003-US34662	20031031
WO 2004041191	A3	20041202		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003286802	A1	20040607	AU 2003-286802	20031031
EP 1565188	A2	20050824	EP 2003-778016	20031031
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003015939	A	20050913	BR 2003-15939	20031031
CN 1732003	A	20060208	CN 2003-80108088	20031031
JP 2006507307	T	20060302	JP 2004-550330	20031031
NZ 540187	A	20080328	NZ 2003-540187	20031031
MX 2005004550	A	20050726	MX 2005-4550	20050428
ZA 2005003469	A	20060830	ZA 2005-3469	20050429

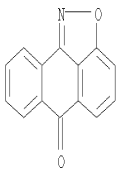
PRIORITY APPLN. INFO.:
US 2002-422896P P 20021031
US 2003-699105 A 20031030
WO 2003-US34662 W 20031031

OTHER SOURCE(S): MARPAT 140:386068
IT 63973-07-9, 6H-Anthra[9,1-cd]isoxazol-6-one 63973-07-9D, 6H-Anthra[9,1-cd]isoxazol-6-one, derivs.
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(JNK inhibitor for treatment, prevention and management of macular degeneration)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



RN 63973-07-9 CAPLUS

CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)

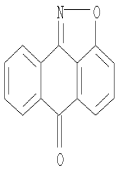


L6 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:372884 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 140:368721
TITLE: Methods of using and compositions comprising a JNK inhibitor for the treatment, prevention, management and/or modification of pain
INVENTOR(S): Zeldis, Jerome B.; Faleck, Herbert; Manning, Donald C.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 35 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040087642	A1	20040506	US 2003-693793	20031023
CA 2503616	A1	20040513	CA 2003-2503616	20031024
WO 2004039325	A2	20040513	WO 2003-US34006	20031024
WO 2004039325	A3	20041111		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003284980	A1	20040525	AU 2003-284980	20031024
AU 2003284980	B2	20080807		
EP 1553951	A2	20050720	EP 2003-779300	20031024
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003015573	A	20050830	BR 2003-15573	20031024
CN 1732004	A	20060208	CN 2003-80107549	20031024
JP 2006511495	T	20060406	JP 2004-548497	20031024
ZA 2005003242	A	20061025	ZA 2005-3242	20031024
NZ 540027	A	20080430	NZ 2003-540027	20031024
MX 2005004180	A	20050920	MX 2005-4180	20050420

PRIORITY APPLN. INFO.:
US 2002-421104P P 20021024
US 2003-693793 A 20031023
WO 2003-US34006 W 20031024

OTHER SOURCE(S): MARPAT 140:368721
IT 63973-07-9, 6H-Anthra[9,1-cd]isoxazol-6-one
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(JNK inhibitor for treatment, prevention, management and/or modification of pain)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



L6 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:972189 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 140:13101
TITLE: Methods of using JNK or MKK inhibitors to modulate cell differentiation and to treat myeloproliferative disorders and myelodysplastic syndromes
INVENTOR(S): Hariri, Robert J.; Stirling, David I.; Zeldis, Jerome B.
PATENT ASSIGNEE(S): Celgene Corporation, USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003102151	A2	20031211	WO 2003-US17319	20030530
WO 2003102151	A3	20050303		
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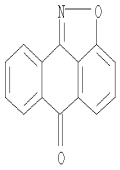
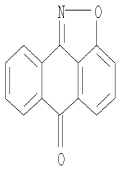
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2488013	A1	20031211	CA 2003-2488013	20030530
AU 2003231950	A1	20031219	AU 2003-231950	20030530
US 20040028660	A1	20040212	US 2003-449248	20030530
EP 1525308	A2	20050427	EP 2003-756349	20030530
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1668733	A	20050914	CN 2003-817267	20030530
JP 2005528105	T	20050922	JP 2004-510393	20030530
MX 2004011851	A	20050331	MX 2004-11851	20041129

PRIORITY APPLN. INFO.:
US 2002-384250P P 20020530
US 2002-434833P P 20021219
WO 2003-US17319 W 20030530

OTHER SOURCE(S): MARPAT 140:13101
IT 63973-07-9, 6H-Anthra[9,1-cd]isoxazol-6-one 63973-07-9D,
6H-Anthra[9,1-cd]isoxazol-6-one, derivs.
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(JNK or MKK inhibitors to modulate cell differentiation and to treat
myeloproliferative disorders and myelodysplastic syndromes)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:950794 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 140:796
TITLE: Methods using JNK inhibitors for treating or
preventing disease-related wasting
INVENTOR(S): Zeldis, Jerome B.
PATENT ASSIGNEE(S): Signal Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003099221	A2	20031204	WO 2003-US16333	20030523
WO 2003099221	A3	20040624		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

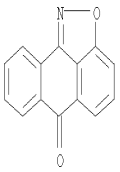
US 20040034084	A1	20040219	US 2003-443263	20030522
CA 2487073	A1	20031204	CA 2003-2487073	20030523
AU 2003256259	A1	20031212	AU 2003-256259	20030523
EP 1507528	A2	20050223	EP 2003-755458	20030523

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

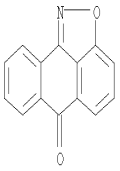
CN 1668299	A	20050914	CN 2003-816699	20030523
JP 2005535594	T	20051124	JP 2004-506748	20030523
NZ 537055	A	20060728	NZ 2003-537055	20030523
MX 2004011599	A	20050727	MX 2004-11599	20041123

PRIORITY APPLN. INFO.:	US 2002-383202P	P 20020524
	US 2003-443263	A 20030522
	WO 2003-US16333	W 20030523

OTHER SOURCE(S): MARPAT 140:796
IT 63973-07-9, 6H-Anthra[9,1-cd]isoxazol-6-one 63973-07-9D,
6H-Anthra[9,1-cd]isoxazol-6-one, derivs.
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(JNK inhibitors for treating or preventing disease-related wasting)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)

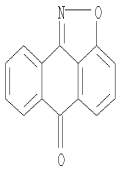


L6 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1978:113354 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 88:113354
ORIGINAL REFERENCE NO.: 88:17699a,17702a
TITLE: Light-sensitive copying composition with synergistic
initiator system
INVENTOR(S): Frass, Werner
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 48 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2558813	A1	19770707	DE 1975-2558813	19751227
DE 2558813	C2	19841031		
BE 849869	A1	19770624	BE 1976-173645	19761224
NL 7614408	A	19770629	NL 1976-14408	19761224
NL 182755	B	19871201		
NL 182755	C	19880502		
CA 1058943	A1	19790724	CA 1976-268737	19761224
GB 1576217	A	19801001	GB 1976-54129	19761224
JP 52082415	A	19770709	JP 1976-160861	19761227
JP 59033893	B	19840818		
FR 2336708	A1	19770722	FR 1976-39131	19761227
FR 2336708	B1	19790309		

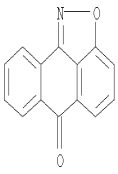
PRIORITY APPLN. INFO.: DE 1975-2558813 A 19751227
IT 63973-07-9
RL: USES (Uses)
(photoinitiator compns. containing, synergistic, for photoimaging compns.)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



L6 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1977:509454 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 87:109454
ORIGINAL REFERENCE NO.: 87:17291a,17294a
TITLE: Light-sensitive copying material containing photoinitiators
INVENTOR(S): Frass, Werner
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 38 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2558812	A1	19770707	DE 1975-2558812	19751227
DE 2558812	C2	19870430		
BE 849868	A1	19770624	BE 1976-173644	19761224
NL 7614410	A	19770629	NL 1976-14410	19761224
GB 1576218	A	19801001	GB 1976-54130	19761224
CA 1088057	A1	19801021	CA 1976-268714	19761224
JP 52083369	A	19770712	JP 1976-160860	19761227
JP 60037456	B	19850826		
FR 2400222	A1	19790309	FR 1976-39132	19761227
FR 2400222	B1	19820226		

PRIORITY APPLN. INFO.: DE 1975-2558812 A 19751227
IT 63973-07-9
RL: USES (Uses)
(photoinitiator, for photoimaging compns. containing ethylenically unsatd. polymerizable compound and binder)
RN 63973-07-9 CAPLUS
CN 6H-Anthra[9,1-cd]isoxazol-6-one (9CI) (CA INDEX NAME)



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ENTER NAME OR (END):stn10591974/l
L# LIST L1-L6 HAS BEEN SAVED AS 'STN10591974/L'

=> d his

     (FILE 'HOME' ENTERED AT 08:29:47 ON 21 JUN 2009)

     FILE 'REGISTRY' ENTERED AT 08:30:00 ON 21 JUN 2009
L1             STRUCTURE UPLOADED
L2           3 S L1 SSS SAM
L3          59 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 08:30:28 ON 21 JUN 2009
L4          21 S L3
L5          10 S L4 AND (PREP/RL OR SPN/RL)
L6          11 S L4 NOT L5
               SAVE ALL STN10591974/L

=> log
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y


     (FILE 'HOME' ENTERED AT 08:29:47 ON 21 JUN 2009)

     FILE 'REGISTRY' ENTERED AT 08:30:00 ON 21 JUN 2009
L1             STRUCTURE UPLOADED
L2           3 SEA SSS SAM L1
L3          59 SEA SSS FUL L1

     FILE 'CAPLUS' ENTERED AT 08:30:28 ON 21 JUN 2009
L4          21 SEA SPE=ON  ABB=ON  PLU=ON  L3
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L5          10 SEA SPE=ON  ABB=ON  PLU=ON  L4 AND (PREP/RL OR SPN/RL)
               D 1-10 IBIB HITSTR
L6          11 SEA SPE=ON  ABB=ON  PLU=ON  L4 NOT L5
               D 1-11 IBIB HITSTR
               SAVE ALL STN10591974/L
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               88.67     274.77

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


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 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  DEC 01  ChemPort single article sales feature unavailable
 NEWS  3  APR 03  CAS coverage of exemplified prophetic substances
                  enhanced
 NEWS  4  APR 07  STN is raising the limits on saved answers
 NEWS  5  APR 24  CA/CAplus now has more comprehensive patent assignee
                  information
 NEWS  6  APR 26  USPATFULL and USPAT2 enhanced with patent
                  assignment/reassignment information
 NEWS  7  APR 28  CAS patent authority coverage expanded
 NEWS  8  APR 28  ENCOMPLIT/ENCOMPLIT2 search fields enhanced
 NEWS  9  APR 28  Limits doubled for structure searching in CAS
                  REGISTRY
 NEWS 10  MAY 08  STN Express, Version 8.4, now available
 NEWS 11  MAY 11  STN on the Web enhanced
 NEWS 12  MAY 11  BEILSTEIN substance information now available on
                  STN Easy
 NEWS 13  MAY 14  DGENE, PCTGEN and USGENE enhanced with increased
                  limits for exact sequence match searches and
                  introduction of free HIT display format
 NEWS 14  MAY 15  INPADOCDB and INPAFAMDB enhanced with Chinese legal
                  status data
 NEWS 15  MAY 28  CAS databases on STN enhanced with NANO super role in
                  records back to 1992
 NEWS 16  JUN 01  CAS REGISTRY Source of Registration (SR) searching
                  enhanced on STN

 NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
              AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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  and other penalties.

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=> file reg
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               0.22       0.22

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provided by InfoChem.

STRUCTURE FILE UPDATES:   19 JUN 2009  HIGHEST RN 1159249-84-9
DICTIONARY FILE UPDATES:  19 JUN 2009  HIGHEST RN 1159249-84-9

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
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http://www.cas.org/support/stngen/stndoc/properties.html

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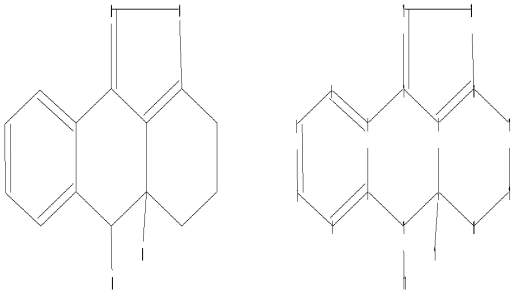

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chain nodes :
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17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
9-18 10-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-15 8-9 8-11 9-10 9-14 11-12
11-16 12-13 13-14 15-16
exact/norm bonds :
4-7 5-10 7-8 7-15 8-9 8-11 9-10 9-14 9-18 10-17 11-12 11-16 12-13 13-14
15-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

L1   STRUCTURE UPLOADED

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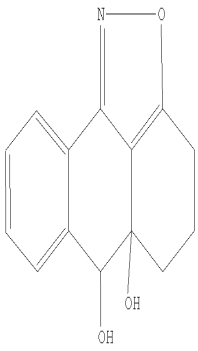
L1   STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 08:41:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   82 TO ITERATE

100.0% PROCESSED   82 ITERATIONS   1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 1097 TO   2183
PROJECTED ANSWERS: 1 TO   80

L2   1 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 08:42:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1664 TO ITERATE

100.0% PROCESSED   1664 ITERATIONS   16 ANSWERS
SEARCH TIME: 00.00.01

L3   16 SEA SSS FUL L1

=> file capl
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                   ENTRY   SESSION
FULL ESTIMATED COST   185.88   186.10

FILE 'CAPLUS' ENTERED AT 08:42:05 ON 21 JUN 2009
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FILE COVERS 1907 - 21 Jun 2009 VOL 150 ISS 26
FILE LAST UPDATED: 19 Jun 2009 (20090619/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

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=> s l3
L4   5 L3

=> d 105 ibib hitstr
     5 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
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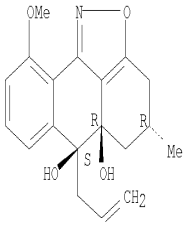
L4   ANSWER 1 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:11627 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 150:237267
TITLE: Isoxazole-assisted direct substitution of the hydroxy
                         group in α-ketols: Introduction of angular
                         substituents in a polycyclic system

AUTHOR(S): Takikawa, Hiroshi; Hikita, Katsuyoshi; Suzuki, Keisuke
CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology, SORST-JST Agency, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2008), 47(51), 9887-9890
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 1116151-27-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(introduction of angular substituents in a polycyclic system via isoxazole-assisted direct substitution of the hydroxy group in α-ketols)
RN 1116151-27-9 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 4,5-dihydro-10-methoxy-4-methyl-6-(2-propen-1-yl)-, (4R,5aR,6S)-rel- (CA INDEX NAME)

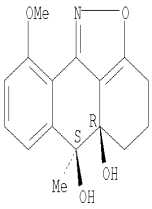
Relative stereochemistry.



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1200735 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 149:576027
TITLE: Formation of α-hydroxy-β-diketones through hydroxylation of isoxazolium salts: stereoselective approach to angular cis-diols in polycyclic systems
AUTHOR(S): Takikawa, Hiroshi; Takada, Akiomi; Hikita, Katsuyoshi; Suzuki, Keisuke
CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology, SORST-JST Agency, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2008), 47(39), 7446-7449
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:576027
IT 1084894-66-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of α-hydroxy-β-diketones through N-methylation of isoxazoles with trimethyloxonium tetrafluoroborate and hydroxylation of isoxazolium salts)
RN 1084894-66-5 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 4,5-dihydro-10-methoxy-6-methyl-, (5aR,6S)-rel- (CA INDEX NAME)

Relative stereochemistry.

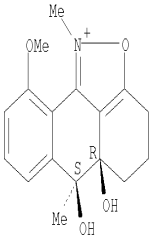


IT 1084894-75-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of α-hydroxy-β-diketones through N-methylation of isoxazoles with trimethyloxonium tetrafluoroborate and hydroxylation of isoxazolium salts)
RN 1084894-75-6 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazolium, 4,5,5a,6-tetrahydro-5a,6-dihydroxy-10-methoxy-1,6-dimethyl-, (5aR,6S)-rel-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

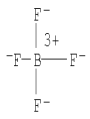
CRN 1084894-74-5
CMF C17 H20 N O4

Relative stereochemistry.



CM 2

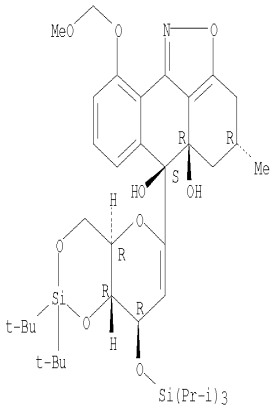
CRN 14874-70-5
CMF B F4
CCI CCS



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

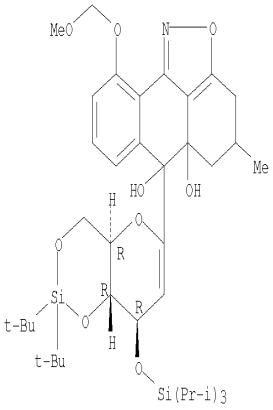
L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:190171 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 148:449823
TITLE: Total synthesis and structure assignment of the anthrone C-glycoside cassialoin
AUTHOR(S): Koyama, Yasuhito; Yamaguchi, Ryo; Suzuki, Keisuke
CORPORATE SOURCE: Department of Chemistry, SORST-JST Agency, Tokyo Institute of Technology, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2008), 47(6), 1084-1087
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:449823
IT 1017858-06-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal structure of; synthesis and structure assignment of the anthrone C-glycoside cassialoin via isoxazole-containing stereogenic α-ketol and a subsequent intramol. redox reaction)
RN 1017858-06-8 CAPLUS
CN D-arabino-Hex-1-enitol, 1,5-anhydro-4,6-O-[bis(1,1-dimethylethyl)silylene]-2-deoxy-1-C-[(4R,5aR,6S)-4,5,5a,6-tetrahydro-5a,6-dihydroxy-10-(methoxymethoxy)-4-methyl-3H-anthra[9,1-cd]isoxazol-6-yl]-3-O-[tris(1-methylethyl)silyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 1018672-95-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and structure assignment of the anthrone C-glycoside cassialoin via isoxazole-containing stereogenic α-ketol and a subsequent intramol. redox reaction)
RN 1018672-95-1 CAPLUS
CN D-arabino-Hex-1-enitol, 1,5-anhydro-4,6-O-[bis(1,1-dimethylethyl)silylene]-2-deoxy-1-C-[4,5,5a,6-tetrahydro-5a,6-dihydroxy-10-(methoxymethoxy)-4-methyl-3H-anthra[9,1-cd]isoxazol-6-yl]-3-O-[tris(1-methylethyl)silyl]- (CA INDEX NAME)

Absolute stereochemistry.



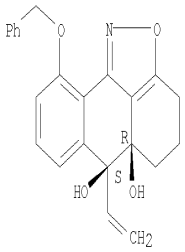
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:546202 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 147:117809
TITLE: Isoxazole-directed pinacol rearrangement: stereocontrolled approach to angular stereogenic centers
AUTHOR(S): Suzuki, Keisuke; Takikawa, Hiroshi; Hachisu, Yoshifumi; Bode, Jeffrey W.
CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology, SORST-JST Agency, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2007), 46(18), 3252-3254
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:117809
IT 943151-36-8P 943151-38-0P 943151-39-1P
943151-44-8P 943151-48-2P 943151-49-3P
943151-50-6P 943151-51-7P 943151-52-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

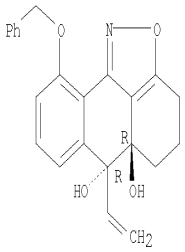
RN 943151-36-8 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 6-ethenyl-4,5-dihydro-10-(phenylmethoxy)-, (5aR,6S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



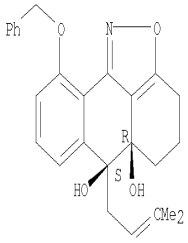
RN 943151-38-0 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 6-ethenyl-4,5-dihydro-10-(phenylmethoxy)-, (5aR,6R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



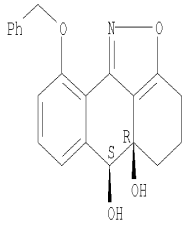
RN 943151-39-1 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 4,5-dihydro-6-(3-methyl-2-buten-1-yl)-10-(phenylmethoxy)-, (5aR,6S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



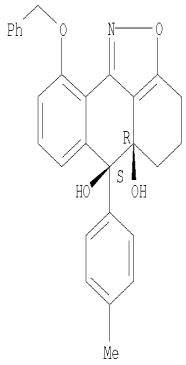
RN 943151-44-8 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 4,5-dihydro-10-(phenylmethoxy)-, (5aR,6S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



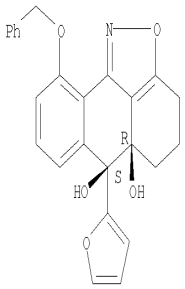
RN 943151-48-2 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 4,5-dihydro-6-(4-methylphenyl)-10-(phenylmethoxy)-, (5aR,6S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



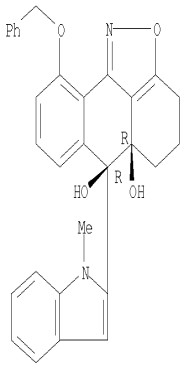
RN 943151-49-3 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 6-(2-furanyl)-4,5-dihydro-10-(phenylmethoxy)-, (5aR,6S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



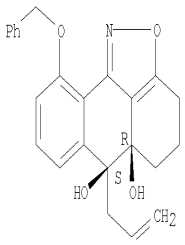
RN 943151-50-6 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 4,5-dihydro-6-(1-methyl-1H-indol-2-yl)-10-(phenylmethoxy)-, (5aR,6R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



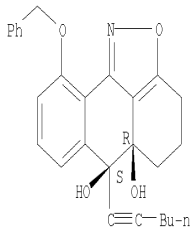
RN 943151-51-7 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 4,5-dihydro-10-(phenylmethoxy)-6-(2-propen-1-yl)-, (5aR,6S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 943151-52-8 CAPLUS
CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 6-(1-hexyn-1-yl)-4,5-dihydro-10-(phenylmethoxy)-, (5aR,6S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1023428 CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER: 143:306299
TITLE: Preparation of polycyclic ketones having anthraisoxazole structure by pinacol rearrangement of diols
INVENTOR(S): Suzuki, Keisuke
PATENT ASSIGNEE(S): Japan Science and Technology Agency, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

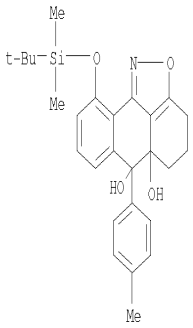
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005255592	A	20050922	JP 2004-67741	20040310
JP 4219289	B2	20090204		
WO 2005095422	A1	20051013	WO 2005-JP4723	20050310
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1724274	A1	20061122	EP 2005-720958	20050310
R: DE, FR, GB				
US 20070149786	A1	20070628	US 2006-591974	20060908

PRIORITY APPLN. INFO.: JP 2004-67741 A 20040310
WO 2005-JP4723 W 20050310
OTHER SOURCE(S): CASREACT 143:306299; MARPAT 143:306299
IT 864951-74-6P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

RN 864951-74-6 CAPLUS

CN 3H-Anthra[9,1-cd]isoxazole-5a,6(6H)-diol, 10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4,5-dihydro-6-(4-methylphenyl)- (9CI) (CA INDEX NAME)



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ANABSTR	- Analytical Abstracts
ANTE	- Abstr. in New Technologies and Eng. 1981 - present
APOLLIT	- APPLIED POLYMERS LITERATURE 1973-present
AQUALINE	- Aqualine 1960 to the present
AQUASCI	- Aquatic Sciences & Fisheries Abstracts 1978-present
AQUIRE	- Acquatic Toxicity Information Retrieval
BABS	- BEILSTEIN Database Abstracts 1980-present
BEILSTEIN	- BEILSTEIN File of Organic Compounds
BIBLIODATA	- GERMAN NATIONAL BIBLIOGRAPHY FROM 1945 - PRESENT
BIOENG	- Biotechnology and Bioengineering database 1982 - pres.
BIOSIS	- The BIOSIS Previews(R)/RN File 1969-present
BIOTECHABS	- Derwent Biotechnology Resource 1982-present
BIOTECHDS	- Derwent Biotechnology Resource 1982-present (Subsc.)
BIOTECHNO	- BIOTECHNOBASE 1980 TO 2003
CA	- The Chemical Abstracts File 1907-present
CABA	- CAB ABSTRACTS 1973-present
CAPLUS	- The Chemical Abstracts Plus File 1907-present
CASREACT	- The Chemical Abstracts Reaction Search Service
CBNB	- Chemical Business NewsBase from 1984-present
CEABA-VTB	- Chem Eng and Biotech Abstr - Verfahrenstechn Ber 1966-
CERAB	- Ceramic Abstracts/World Ceramic Abstracts from 1975
CHEMCATS	- CHEMICAL CATALOGS ONLINE 1993-to the present
CHEMINFORMRX	- The CHEMINFORMRX Reaction Search Service
CHEMLIST	- Regulated Chemicals Listing
CHEMSAFE	- CHEMSAFE - chemical safety information
CIN	- The Chemical Industry Notes File for 1974-present
CIVILENG	- Civil Engineering Abstracts 1966 to the present
COMPENDEX	- COMPENDEX*PLUS File from 1970 - present
COMPUAB	- Computer & Information Systems Abstracts 1981-present
COMPUSCIENCE	- COMPUTERSCIENCE FROM 1972-2002
CONFSCI	- Conference Papers Index from 1973-present
COPPERLIT	- Copper Literature Database
CORROSION	- Corrosion Abstracts 1980 to the present
CROPB	- Derwent Crop Protection File 1968 - 1984
CROPR	- Derwent Crop Protection Registry
CROPU	- DERWENT CROP PROTECTION FILE 1985 - 2003
CSCHEM	- ChemSources - USA and International (Chemicals)
CSCORP	- ChemSources - USA and International (Company Directory
CSNB	- Chemical Safety News Base from 1981-present
DDFB	- Derwent Drug File, Backfile 1964 - 1982
DDFU	- Derwent Drug File from 1983 - present
DETHERM	- DETHERM-DECHEMA thermophysical property database
DGENE	- Derwent Geneseq Database 1981 - present
DISSABS	- Dissertation Abstracts from 1861 to present
DJSMDS	- Derwent Reaction Search Service DJSM (Subscribers)
DJSMONLINE	- Derwent Reaction Search Service DJSM
DKF	- The German Automotive Engineering Database 1974-date
DRUGB	- Derwent Drug File, Backfile 1964 - 1982 (Subscribers)
DRUGMONOG	- IMS Product Monographs (Approved Pharm. Industry Users
DRUGMONOG2	- IMS Product Monographs
DRUGU	- Derwent Drug File from 1983-present (Subscribers)
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EMA	- Engineered Materials Abstracts File from 1986-present
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ENCOMPPAT2	- EnCompass Patent File 1964-Present (Non-Supporters)
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FSTA - Food Science Technology Abstracts from 1969 - present
GBFULL - United Kingdom (GB) Patents Full Text from 1979 - pres
GENBANK - Genetic Sequence Data Bank
GEOREF - Geological Reference File 1785-present
GMELIN97 - Gmelin Handb. of Inorg. Chem. + Sci. Publ. 1817-1997
HCA - CA File with hour-based pricing
HCAPLUS - CAPLUS File with hour-based pricing
HCHEMLIST - Regulated Chemicals Listing with hour-based pricing
HCIN - The CIN File for 1974-present with hour-based pricing
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HSDB - Hazardous Substances Databank
ICONDA - International Construction Database from 1976-present
ICSD - ICSD - Inorganic Crystal Structure Data File
IFICDB - The IFI Comprehensive Database from 1950-present
IFICLS - The IFI Current Patent Legal Status Database
IFIPAT - The IFI Patent Database from 1950-present
IFIREF - The IFI Uniterm and U.S. Class Reference File
IFIUDB - The IFI Uniterm Database from 1950-present
IMSCOPROFILE - IMS Company Profiles 1995-present
IMSCOSEARCH - IMS Company Search
IMSDRUGNEWS - IMS Drug News 1991-present
IMSPATENTS - IMS LifeCycle, Patent Focus with Patent Family Data
IMSPRODUCT - IMS LifeCycle, New Product Focus from 1982-present
IMSRESEARCH - IMS LifeCycle, R&D Focus 1977-present
INFODATA - Information Science and Work from 1976 to present
INIS - International Nuclear Information System 1970-present
INPADOCDB - The Intern. Patent Documentation Database 1836-pres.
INPAFAMDB - International Patent Family Database 1836-pres.
INSPEC - INSPEC file from 1898 - present
INSPHYS - INSPHYS - Inspec Phys Supplement Backfile (1979 - 1994
IPA - International Pharmaceutical Abstracts 1970-present
ITRD - International Transport Research Documentation 1972-da
JAPIO - JAPIO - Japanese Patents from 1976 - present
KOREAPAT - Korean Patent Abstracts Database from 1979 - present
KOSMET - Cosmetic & Perfume Science & Technology 1968-present
LBIBLIO - Bibliodata learning File
LCA - The CA Learning File
LCASREACT - The CAS Reaction Search Service Learning File
LDRUG - Derwent Drug Learn File
LEMBASE - The EMBASE Learning File
LIFESCI - CSA Life Sciences Collection from 1978-present
LINPADOCDB - Learning INPADOCDB File
LINPAFAMDB - Learning INPAFAMDB File
LINSPEC - Learning INSPEC File
LISA - Library and Information Science Abstracts 1969 - pres.
LITALERT - The Patent Litigation Database from 1973 - present
LMARPAT - The CAS Patent Markush Learning File
LMEDLINE - The MEDLINE Learning File
LPATDPA - The PATDPA Learning File
LPCI - Patents Citation Index Learning File
LREGISTRY - The Registry Learning File.
LWPI - Derwent World Patents Index Learning File
MARPAT - The CAS Patent Markush File 1988-present
MATBUS - Materials Business File from 1983-present
MDF - Metals Datafile
MECHENG - Mechanical and Transportation Eng. Abs. 1966-
MEDLINE - MEDlars onLINE File from 1960 - present
METADEX - METADEX File from 1966-present
MRCK - The Merck Index Online (SM)
MSDS-CCOHS - CCOHS Material Safety Data Sheets
MSDS-OHS - Material Safety Data Sheets - OHS
NAPRALERT - Natural Products Alert Database
NLDB - Newsletter Database from 1988 - present
NTIS - U.S.Government Reports Announcements 1964-present
NUTRACEUT - Nutraceuticals International 1996 to the present
OCEAN - Oceanic Abstracts from 1964 - current
PASCAL - PASCAL 1977 to the present
PATDD - East German Patents from 1982-present
PATDPA - The German Patent Database from 1968-present
PATDPAFULL - The German Full-Text Patent Database from 1987-present
PATDPASPC - German SPC for Drugs and Plant Protecting Agents 1992-
PATIPC - International Patent Classification and Catchword Inde
PCI - PATENTS CITATION INDEX 1973 TO PRESENT
PCTFULL - WIPO/PCT Patents Full Text 1978 to the present
PCTGEN - PCTGEN: World Patent Application Biosequences
PHAR - Pharmaprojects drug development status file
PHARMAML - Pharma Marketletter 1992 to the present
PHIN - Pharmaceutical & Healthcare Industry News Archive 1980
PIRA - PIRA & PAPERBASE Database from 1975
POLLUAB - Pollution Abstracts from 1970-present
PROMT - PROMT from 1978 - present
PROUSDDR - Drug Data Report from Prous Science
PS - Pharmaceutical Substances
RAPRA - Rubber, Plastics, Polymer Composites 1972 - present
RDISCLOSURE - Research Disclosure 1960 to the present
REGISTRY - The CAS Registry File of substances
RSWB - Regional planning and building construction
RTECS - Registry of Toxic Effects of Chemical Substances
RUSSIAPAT - RUSSIAN PATENT ABSTRACTS DATABASE FROM 1924 - PRESENT
SCISEARCH - ISI Science Citation Index from 1974 - present
SOFIS - Social Science Research Information System 1997-2006
SOLIDSTATE - Solid State and Superconductivity Abstracts from 1981
SOLIS - German literature in social sciences 1945-present
SPECINFO - Spectral Database Information System
STNGUIDE - Descriptive information about STN databases
STNMAIL - STN Electronic Mail Service
SYNTHLINE - Synthline Drug Synthesis Database 1984-present
TEMA - TEMA: Technology and Management 1990 to the present
TEXTILETECH - Textile Technology Digest from 1978 to the present
TOXCENTER - Toxicology Center from 1907 - present
TRIBO - TRIBOLOGY INDEX (Friction,Wear,Lubrication) 1972-pres.
TULSA - Petroleum Abstracts 1965-present
TULSA2 - Petroleum Abstracts 1965-present (Non-subscribers)
UFORDAT - Environment Research in Progress from 1974 - present
ULIDAT - Environmental Literature from 1976-present
USAN - USAN - United States Adopted Names
USGENE - The USPTO Genetic Sequence Database
USPAT2 - U.S. Patents Latest Publications from 2001 - present
USPATFULL - U.S. Patents Original Publications from 1971 - present
USPATOLD - U.S. PATENTS 1790-1971
VETB - Derwent Veterinary Drug File 1968 - 1982
VETU - Derwent Veterinary Drug File 1983 - 2001
WATER - Water Resource Abstracts 1967 to the present
WELDASEARCH - Weldasearch 1967 to the present
WPIDS - Derwent World Patents Index 1963 - present (Subscr.)
WPIFV - WPIFV - DERWENT WORLD PATENT INDEX FIRST VIEW
WPINDEX - Derwent World Patents Index 1963 - present
WPIX - DERWENT WPI WITH EXTENSION ABSTRACTS 1963 - PRESENT
WSCA - World Surface Coatings Abstracts 1976 - present

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 WTEXTILES    - WORLD TEXTILES 1970 TO THE PRESENT
 ZCA          - CA File with zero connect hour pricing
 ZCAPLUS      - CAPLUS File with zero connect hour pricing
 ZREGISTRY    - Zero connect hour REGISTRY

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for a general description of the file.  Enter "HELP DIRECTORY" for a
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sheet is also available for the file in STNGUIDE.  Enter "FILE
STNGUIDE" at an arrow prompt (=>), then search the file name in the
/DBN search field.  You can then display the search fields, display
fields, file content, sources, etc.

All files are available for multifile searching except HOME,
STNGUIDE, STNMAIL, and the Learning Files.

=> file capl uspatfull dissabs
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                  23.95     210.05

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FILE 'DISSABS' ENTERED AT 08:47:32 ON 21 JUN 2009
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=> s pinacol rearrangement
L5         814 PINACOL REARRANGEMENT

=> s l5 (L) polycyclic or multicyclic
L6        3418 L5 (L) POLYCYCLIC OR MULTICYCLIC

=> s pinacol rearrangement (L) polycyclic
L7          33 PINACOL REARRANGEMENT (L) POLYCYCLIC

=> dup rem l7
PROCESSING COMPLETED FOR L7
L8           33 DUP REM L7 (0 DUPLICATES REMOVED)

=> s pinacol rearrangement/ti
L9         240 PINACOL REARRANGEMENT/TI

=> s l9 and l7
L10          2 L9 AND L7

=> d 1-2 ibib abs

L10  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        2007:546202  CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER:         147:117809
TITLE:                   Isoxazole-directed pinacol
                         rearrangement: stereocontrolled approach to
                         angular stereogenic centers
AUTHOR(S):               Suzuki, Keisuke; Takikawa, Hiroshi; Hachisu,
                         Yoshifumi; Bode, Jeffrey W.
CORPORATE SOURCE:        Department of Chemistry, Tokyo Institute of
                         Technology, SORST-JST Agency, 2-12-1 O-okayama,
                         Meguro-ku, Tokyo, 152-8551, Japan
SOURCE:                  Angewandte Chemie, International Edition (2007),
                         46(18), 3252-3254
                         CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER:               Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE:           Journal
LANGUAGE:                English
OTHER SOURCE(S):         CASREACT 147:117809
AB   Underappreciated and neglected, isoxazoles are extremely good at
     stabilizing α cations.  This ability is exploited in a method for
     the stereocontrolled introduction of angular substituents as found in
     polyketide-derived polycyclic natural products, such as 1.  In a
     two-step process, the stereoselective addition of a nucleophile to the ketol
     2 is followed by a regio- and stereospecific pinacol
     rearrangement.  Bn = benzyl; R = allyl, aryl, heteroaryl, vinyl.
REFERENCE COUNT:         38    THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10  ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        2005:1023428  CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER:         143:306299
TITLE:                   Preparation of polycyclic ketones having
                         anthraisoxazole structure by pinacol
                         rearrangement of diols
INVENTOR(S):             Suzuki, Keisuke
PATENT ASSIGNEE(S):      Japan Science and Technology Agency, Japan
SOURCE:                  Jpn. Kokai Tokkyo Koho, 19 pp.
                         CODEN: JKXXAF
DOCUMENT TYPE:           Patent
LANGUAGE:                Japanese
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     --------------      ----   --------    -------------------    --------
     JP 2005255592        A     20050922    JP 2004-67741          20040310
     JP 4219289           B2    20090204
     WO 2005095422        A1    20051013    WO 2005-JP4723         20050310
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
     EP 1724274           A1    20061122    EP 2005-720958         20050310
         R:  DE, FR, GB
     US 20070149786       A1    20070628    US 2006-591974         20060908
PRIORITY APPLN. INFO.:                       JP 2004-67741      A  20040310
                                             WO 2005-JP4723     W  20050310
OTHER SOURCE(S):         CASREACT 143:306299; MARPAT 143:306299
GI
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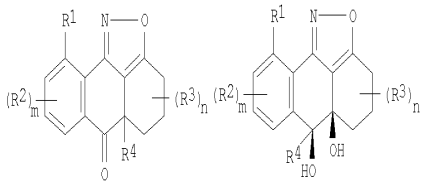
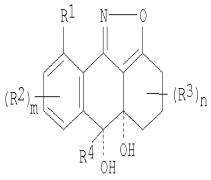


I

II



III

AB Polycyclic ketones I [R1 = H, OH, halo, (un)substituted silyloxy, (un)substituted C1-10 alkoxy, C1-20 hydrocarbyl; R2 = halo, OH, cyano, NO2, (un)substituted amino, (un)substituted C1-10 alkoxy, (un)substituted 5-7-membered heterocycle, etc.; R3 = halo, OH, (un)substituted C1-10 alkoxycarbonyl, (un)substituted C6-20 hydrocarbyl, etc.; 2 adjacent R2s or 2 R3s may form (un)substituted 4-6-membered ring; R4 = H, halo, (un)substituted amino, (un)substituted Ph, etc.; m = 0-3; n = 0-6], useful as intermediates for drugs, agrochems., dyes, etc., are prepared by treating optically-active alcs. II or III (R1-R4, m, n = same as above) under an acidic condition, preferably in the presence of catalysts such as Lewis acids, protonic acids, etc. II or III may be prepared by reacting I (R4 = OH; R1-R3, m, n = same as above) with R4M (R4 = any group given in I; M = metal). Thus, a THF solution of I (R1 = OSiMe2CMe3, R2 = R3 = H, R4 = OH) was added dropwise to a mixture of a THF solution of p-MeC6H4Li, in situ prepared from 4-MeC6H4Br and BuLi, over 10 min and the reaction mixture was stirred for 5 min to give 92% II (or III) (R1 = OSiMe2CMe3, R2 = R3 = H, R4 = 4-C6H4Me). This was treated with a CH2Cl2 solution of BF3.Et2O under stirring for 30 min to give 99% I (R1 = OSiMe2CMe3, R2 = R3 = H, R4 = 4-C6H4Me).

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=> s pinacol rearrangement/ab
L11        407 PINACOL REARRANGEMENT/AB

=> s l11 and l9
L12        110 L11 AND L9

=> s l11 and l7
L13          5 L11 AND L7

=> s l13 not l10
L14          4 L13 NOT L10
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=> d 1-4 ibib abs

L14  ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        2004:658627  CAPLUS <<LOGINID::20090621>>
TITLE:                   Progress toward the total syntheses of the polycyclic
                         terpenes bacchopetiolone and providencin
AUTHOR(S):               Wood, John L.; Drutu, Ioana; Berube, Amelie
CORPORATE SOURCE:        Department of Chemistry, Yale University, New Haven,
                         CT, 06520-8107, USA
SOURCE:                  Abstracts of Papers, 228th ACS National Meeting,
                         Philadelphia, PA, United States, August 22-26, 2004
                         (2004), ORGN-362.  American Chemical Society:
                         Washington, D. C.
                         CODEN: 69FTZ8
DOCUMENT TYPE:           Conference; Meeting Abstract
LANGUAGE:                English
AB   Progress toward the total syntheses of the complex polycyclic
     terpenes will be presented.  The key transformations in these syntheses
     include a tandem phenolic oxidation/Diels-Alder dimerization for
     bacchopetiolone and a cyclopropane ring expansion via a Pinacol
     rearrangement for providencin.

L14  ANSWER 2 OF 4  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        1957:25591  CAPLUS <<LOGINID::20090621>>
DOCUMENT NUMBER:         51:25591
ORIGINAL REFERENCE NO.:  51:5099h-i,5100a
TITLE:                   Aconite alkaloids. VIII. Identity of delphelatine with
                         eldeline
AUTHOR(S):               Kuzovkov, A. D.
CORPORATE SOURCE:        S. Ordzhonikidze All-Union Chem. Pharm. Research
                         Inst., Moscow
SOURCE:                  Zhurnal Obshchei Khimii (1956), 26, 2063-6
                         CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE:           Journal
LANGUAGE:                Unavailable
AB   cf. C.A. 50, 13965d.  Examination of properties of eldeline and delphelatine
     (cf. Feofilaktov and Alekseeva, C.A. 49, 5499a; Rabinovich, C.A. 47,
     9336e) showed that the two alkaloids are identical; infrared absorption
     spectra also prove their identity (these are reproduced).  The name
     eldeline is suggested for future use.  The empirical formula of the
     alkaloid suggested by Rabinovich agrees with analytical data.  Heating the
     alkaloid (80 g.) with 40 g. phloroglucinol in 4 l. HCl 2 hrs. at
     80-90° gave a product of hydrolysis of the methylenedioxy group.
     This substance (I), named demethyleneeldeline, C24H3907N, m.
     106-8°, [α]D 32° (EtOH); HCl salt hemihydrate, decompose
     230-1°, [α]D 7.94° (EtOH); HBr salt, decompose
     198-9°.  I heated with HI-red P and the crude products refluxed 5
     hrs. with Zn-HCl gave an oxo compound, C21H3104N, m. 207-8.5°,
     [α]D 53.8° (EtOH); HBr salt, m. 274-6°; its infrared
     spectrum shows an oxo band in a 6-membered ring, absolute maximum 1725 cm.-1,
as
     well as an HO band at 3565 cm.-1  This ketone is possibly formed by
     pinacol rearrangement of I which apparently contains a
     glycol group.  I heated with Se 8 hrs. at 320-40° gave a
     polycyclic aromatic hydrocarbon, an oil, which gives a
     trinitrobenzoate complex, m. 100-2°.

L14  ANSWER 3 OF 4  DISSABS COPYRIGHT (C) 2009 ProQuest Information and
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ACCESSION NUMBER:   2007:76336  DISSABS   Order Number: AAIMR25798
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TITLE: Prins-pinacol synthesis of a variety of highly functionalized bicyclo[4.n.1]alkanones
AUTHOR: Lavigne, Roch M. A. [M.Sc.]
CORPORATE SOURCE: University of Ottawa (Canada) (0918)
SOURCE: Masters Abstracts International, (2006) Vol. 45, No. 5, p. 2496. Order No.: AAIMR25798. 344 pages.
ISBN: 978-0-494-25798-2.
DOCUMENT TYPE: Dissertation
FILE SEGMENT: MAI
LANGUAGE: English
ENTRY DATE: Entered STN: 20071026
Last Updated on STN: 20071026

AB Bridged ring cores possessing quaternary carbon centers adjacent to a bridged ketone constitute challenging structures in synthesis. Therefore, this thesis explores the development of the first Prins-pinacol synthesis of cis-fused bicyclo[4,n,1]alkanones. The reaction conditions were optimized for the rearrangement of bicyclo[4.4.0]decanes and the effect of different diol protecting groups was explored, as well as the effect of substitution at the C4 and the C5 position. The rearrangement of bicyclo[5.4.0]undecane and bicyclo[5.3.0]decanes was also investigated in order to achieve the formation of bicyclic ketones with various ring sizes. Finally, the Prins-pinacol rearrangement was coupled with an ionic Diels-Alder reaction in order to achieve the rapid synthesis of highly functionalized polycyclic bridgehead ketones.

L14 ANSWER 4 OF 4 DISSABS COPYRIGHT (C) 2009 ProQuest Information and Learning Company; All Rights Reserved on STN
ACCESSION NUMBER: 94:31182 DISSABS Order Number: AAR9418352
TITLE: TETRAHYDROPYRAN AND TETRAHYDROFURAN SYNTHESES VIA RADICAL AND ANIONIC CYCLIZATION AND SYNTHETIC EFFORTS TOWARDS AVENACIOLIDE, ISOAVENACIOLIDE AND HALICHONDRIN B
AUTHOR: JUNG, KYUNG WOON [PH.D.]; BURKE, STEVEN D. [advisor]
CORPORATE SOURCE: THE UNIVERSITY OF WISCONSIN - MADISON (0262)
SOURCE: Dissertation Abstracts International, (1994) Vol. 55, No. 3B, p. 903. Order No.: AAR9418352. 562 pages.
DOCUMENT TYPE: Dissertation
FILE SEGMENT: DAI
LANGUAGE: English
ENTRY DATE: Entered STN: 19940829
Last Updated on STN: 19940829

AB As a stereochemically complementary method to the dioxanone-to-dihydropyran route developed in the Burke laboratories, highly stereoselective syntheses of anti 2,3-disubstituted tetrahydropyrans were accomplished utilizing intramolecular radical cyclization, featuring captodative stabilization and late, tight transition states.

In an extended study, 2,3-disubstituted tetrahydrofurans were synthesized using the same technique as in the tetrahydropyran syntheses, where anti diastereomers were obtained as the dominant product. In addition, anionic cyclizations of appropriate acyclic precursors resulted in the highly stereoselective syntheses of anti 2,3-disubstituted tetrahydrofurans.

The syntheses of tetrahydrofurans were directly applied to the stereo-divergent formal total syntheses of two natural mold metabolites, avenaciolide and isoavenaciolide. The salient features involved in the synthesis included the intramolecular Pummerer rearrangement and C-allylation.

The last issue in this dissertation is focused on the synthesis of the C(1)-C(14) subunit of halichondrin B, a tubulin-based antimitotic anticancer agent. Included in the synthesis are a pinacol rearrangement, intramolecular Michael addition, and a one-pot multistep conversion leading to the formation of the lipophilic polycyclic ketal, the C(8)-C(14) substructure of halichondrin B.

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 19, 2009 (20090619/UP).

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'AB' IS NOT A VALID FIELD CODE
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             0 PINACOL REARRANGEMENT (L) POLYCYCLIC
             0 PINACOL REARRANGEMENT/TI
             0 PINACOL
             0 REARRANGEMENT
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               (PINACOL(W)REARRANGEMENT)
             0 POLYCYCLIC
             0 PINACOL REARRANGEMENT (L) POLYCYCLIC
             0 PINACOL REARRANGEMENT/AB
             0 PINACOL
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             0 POLYCYCLIC
             0 PINACOL REARRANGEMENT (L) POLYCYCLIC
             0 PINACOL REARRANGEMENT/TI
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               (PINACOL(W)REARRANGEMENT)
             0 POLYCYCLIC
             0 PINACOL REARRANGEMENT (L) POLYCYCLIC
L15          0 L7 NOT (L10 OR L14)

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             0 POLYCYCLIC
             0 PINACOL REARRANGEMENT (L) POLYCYCLIC
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L16         0 L7 NOT L10

=> d l7 1-33 abs
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS, USPATFULL, DISSABS' - CONTINUE? (Y)/N:y
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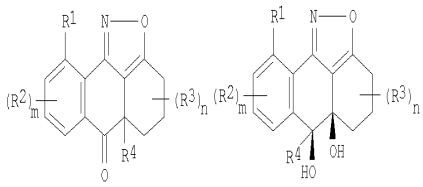
L7 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2009 ACS on STN

AB Underappreciated and neglected, isoxazoles are extremely good at stabilizing α cations. This ability is exploited in a method for the stereocontrolled introduction of angular substituents as found in polyketide-derived polycyclic natural products, such as 1. In a two-step process, the stereoselective addition of a nucleophile to the ketol 2 is followed by a regio- and stereospecific pinacol rearrangement. Bn = benzyl; R = allyl, aryl, heteroaryl, vinyl.

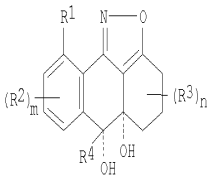
L7 ANSWER 2 OF 33 CAPLUS COPYRIGHT 2009 ACS on STN

GI



I

II



III

AB Polycyclic ketones I [R1 = H, OH, halo, (un)substituted silyloxy, (un)substituted C1-10 alkoxy, C1-20 hydrocarbyl; R2 = halo, OH, cyano, NO2, (un)substituted amino, (un)substituted C1-10 alkoxy, (un)substituted 5-7-membered heterocycle, etc.; R3 = halo, OH, (un)substituted C1-10 alkoxycarbonyl, (un)substituted C6-20 hydrocarbyl, etc.; 2 adjacent R2s or 2 R3s may form (un)substituted 4-6-membered ring; R4 = H, halo, (un)substituted amino, (un)substituted Ph, etc.; m = 0-3; n = 0-6], useful as intermediates for drugs, agrochems., dyes, etc., are prepared by treating optically-active alcs. II or III (R1-R4, m, n = same as above) under an acidic condition, preferably in the presence of catalysts such as Lewis acids, protonic acids, etc. II or III may be prepared by reacting I (R4 = OH; R1-R3, m, n = same as above) with R4M (R4 = any group given in I; M = metal). Thus, a THF solution of I (R1 = OSiMe2CMe3, R2 = R3 = H, R4 = OH) was added dropwise to a mixture of a THF solution of p-MeC6H4Li, in situ prepared from 4-MeC6H4Br and BuLi, over 10 min and the reaction mixture was stirred for 5 min to give 92% II (or III) (R1 = OSiMe2CMe3, R2 = R3 = H, R4 = 4-C6H4Me). This was treated with a CH2Cl2 solution of BF3.Et2O under stirring for 30 min to give 99% I (R1 = OSiMe2CMe3, R2 = R3 = H, R4 = 4-C6H4Me).

L7 ANSWER 3 OF 33 CAPLUS COPYRIGHT 2009 ACS on STN

AB Progress toward the total syntheses of the complex polycyclic terpenes will be presented. The key transformations in these syntheses include a tandem phenolic oxidation/Diels-Alder dimerization for bacchopetiolone and a cyclopropane ring expansion via a Pinacol rearrangement for providencin.

L7 ANSWER 4 OF 33 CAPLUS COPYRIGHT 2009 ACS on STN

AB cf. C.A. 50, 13965d. Examination of properties of eldeline and delphelatine (cf. Feofilaktov and Alekseeva, C.A. 49, 5499a; Rabinovich, C.A. 47, 9336e) showed that the two alkaloids are identical; infrared absorption spectra also prove their identity (these are reproduced). The name eldeline is suggested for future use. The empirical formula of the alkaloid suggested by Rabinovich agrees with analytical data. Heating the alkaloid (80 g.) with 40 g. phloroglucinol in 4 l. HCl 2 hrs. at 80-90° gave a product of hydrolysis of the methylenedioxy group. This substance (I), named demethyleneeldeline, C24H39O7N, m. 106-8°, [α]D 32° (EtOH); HCl salt hemihydrate, decompose 230-1°, [α]D 7.94° (EtOH); HBr salt, decompose 198-9°. I heated with HI-red P and the crude products refluxed 5 hrs. with Zn-HCl gave an oxo compound, C21H31O4N, m. 207-8.5°, [α]D 53.8° (EtOH); HBr salt, m. 274-6°; its infrared spectrum shows an oxo band in a 6-membered ring, absolute maximum 1725 cm.-1, as well as an HO band at 3565 cm.-1 This ketone is possibly formed by pinacol rearrangement of I which apparently contains a glycol group. I heated with Se 8 hrs. at 320-40° gave a polycyclic aromatic hydrocarbon, an oil, which gives a trinitrobenzoate complex, m. 100-2°.

L7 ANSWER 5 OF 33 USPATFULL on STN

AB One aspect of the present invention relates to ionic liquids comprising a pendant Bronsted-acidic group, e.g., a sulfonic acid group. Another aspect of the present invention relates to the use of an ionic liquid comprising a pendant Bronsted-acidic group to catalyze a Bronsted-acid-catalyzed chemical reaction. A third aspect of the present invention relates to ionic liquids comprising a pendant nucleophilic group, e.g., an amine. Still another aspect of the present invention relates to the use of an ionic liquid comprising a pendant nucleophilic group to catalyze a nucleophile-assisted chemical reaction. A fifth aspect of the present invention relates to the use of an ionic liquid comprising a pendant nucleophilic group to remove a gaseous impurity, e.g., carbon dioxide, from a gas, e.g., sour natural gas.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 6 OF 33 USPATFULL on STN

AB Disclosed are cationic photocurable compositions with improved shelf life stability. The thermally stable compositions comprise at least one cationically polymerizable compound, for example an epoxy compound, at least one onium salt photoinitiator and at least one compound selected from the group consisting of the organic phosphorus stabilizers and the hindered nitroxyl stabilizers. Also disclosed is a cationic photoinitiator composition comprising at least one onium salt photoinitiator and at least one compound selected from the group consisting of the organic phosphorus stabilizers and the hindered nitroxyl stabilizers.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 7 OF 33 USPATFULL on STN

AB A method for making an inorganic structure including: (a) applying a photoreactive composition to a substrate, wherein the composition includes: a reactive species, a photoinitiator system, and a plurality of substantially inorganic colloidal particles, wherein the particles have an average particle size of less than about 300 nm; (b) photopatterning the composition to define a structure; and (c) subjecting the structure to elevated temperature for a time sufficient to pyrolyze the reactive species and to at least partially fuse the particles.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 8 OF 33 USPATFULL on STN

AB The present invention provides a water-soluble transition metal-diamine complex which can be easily separated from reaction products through liquid separation, etc. and is recycleable; an optically active diamine compound constituting the ligand of the complex; and a catalyst for asymmetric synthesis which comprises these. The present invention relates to a water-soluble optically active transition metal-diamine complex represented by the formula (2): ##STR1## [wherein R.sup.1 and R.sup.2 each represents hydrogen, a hydrocarbon group, --SO.sub.2R.sup.13 (wherein R.sup.13 is a hydrocarbon group, substituted amino, etc.), etc.; R.sup.3 to R.sup.12 each represents hydrogen, a hydrocarbon group, alkoxy, substituted amino, etc.; M represents a transition metal; X represents halogen; L represents a ligand; and * indicates an asymmetric carbon atom; provided that at least one of R.sup.3 to R.sup.7 and R.sup.8 to R.sup.12 is substituted amino], a catalyst for asymmetric synthesis containing the complex, and a process for producing an optically active alcohol, which comprises using the catalyst to asymmetrically reduce a ketone.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 9 OF 33 USPATFULL on STN

AB The application discloses novel synthetic compounds, modeled after unique toxins extracted from the marine invertebrate Diazona angulata useful in the treatment abnormal cell mitosis. The application also discloses novel methods for synthesis of these compounds and methods of using these compounds.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 10 OF 33 USPATFULL on STN

AB There is provided a novel fluorine-containing polymer having an acid-reactive group which has a high transparency against energy rays (radioactive rays) in a vacuum ultraviolet region (157 nm), and further there are provided a material for fluorine-containing base polymer prepared from the polymer and suitable for a photoresist and a chemically amplifying type resist composition obtained therefrom. The polymer has a number average molecular weight of from 1,000 to 1,000,000 and represented by the formula: -(M1)-(M2)-(A)-, wherein M1 is a structural unit having an acid-labile or acid-degradable functional group, M2 is a structural unit of fluorine-containing acryl ester, A is a structural unit derived from other copolymerizable monomer, the percent by mole ratio M1/M2 is 1 to 99/99 to 1 and the polymer comprises from 1 to 99% by mole of the structural unit M1, from 1 to 99% by mole of the structural unit M2 and from 0 to 98% by mole of the structural unit A1. The material for fluorine-containing base polymer comprises a fluorine-containing polymer having an acid-reactive group such as the above-mentioned polymer and is suitable for a photoresist, and the chemically amplifying type resist composition is obtained from those polymer and material.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 11 OF 33 USPATFULL on STN

AB There is provided a process for preparing a fluorine-containing polymer for resist which is excellent in transparency in a vacuum ultraviolet region, comprises a structural unit derived from a fluorine-containing ethylenic monomer and/or a structural unit derived from a monomer which can provide an aliphatic ring structure in the polymer trunk chain and may have a fluorine atom, and has an acid-reactive group Y.sup.1 reacting with an acid or a group Y.sup.2 which can be converted to the acid-reactive group Y.sup.1, in which the fluorine-containing ethylenic monomer and/or the monomer which can provide an aliphatic ring structure in the polymer trunk chain are subjected to radical polymerization by using an organic peroxide represented by the formula (1): ##STR1## wherein R.sup.50 and R.sup.51 are the same or different and each is a hydrocarbon group having 1 to 30 carbon atoms which may have ether bond (an atom at an end of bond is not oxygen atom); p1 and p2 are the same or different and each is 0 or 1; p3 is 1 or 2, and also there is provided a photoresist composition comprising the obtained polymer. The fluorine-containing polymer is excellent in transparency in a vacuum ultraviolet region, and can form an ultra fine pattern as a polymer for a photoresist, particularly for a F2 resist.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 12 OF 33 USPATFULL on STN

AB Disclosed are cationic photocurable compositions with improved shelf life stability. The thermally stable compositions comprise at least one cationically polymerizable compound, for example an epoxy compound, at least one onium salt photoinitiator and at least one compound selected from the group consisting of the organic phosphorus stabilizers and the hindered nitroxyl stabilizers. Also disclosed is a cationic photoinitiator composition comprising at least one onium salt photoinitiator and at least one compound selected from the group consisting of the organic phosphorus stabilizers and the hindered nitroxyl stabilizers.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 13 OF 33 USPATFULL on STN

AB A process for producing photonic crystals comprises (a) providing a substantially inorganic photoreactive composition; (b) exposing, using a multibeam interference technique involving at least three beams, at least a portion of the photoreactive composition to radiation of appropriate wavelength, spatial distribution, and intensity to produce a

two-dimensional or three-dimensional periodic pattern of reacted and non-reacted portions of the photoreactive composition; and (c) removing the non-reacted portion or the reacted portion of the photoreactive composition to form interstitial void space.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 14 OF 33 USPATFULL on STN
AB A method for making an inorganic structure including:

(a) applying a photoreactive composition to a substrate, wherein the composition includes:

a reactive species,

a photoinitiator system, and

a plurality of substantially inorganic colloidal particles, wherein the particles have an average particle size of less than about 300 nm;

(b) photopatterning the composition to define a structure; and

(c) subjecting the structure to elevated temperature for a time sufficient to pyrolyze the reactive species and to at least partially fuse the particles.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 15 OF 33 USPATFULL on STN
AB A method of multiphoton photosensitizing comprises

(a) providing a multiphoton-activatable, photoreactive composition comprising

(1) at least one reactive species that is capable of undergoing an acid- or radical-initiated chemical reaction, and

(2) a photoinitiator system comprising photochemically-effective amounts of

(i) at least one type of semiconductor nanoparticle that has at least one electronic excited state that is accessible by absorption of two or more photons, and

(ii) a composition that is capable of interacting with the excited state of the semiconductor nanoparticle to form at least one reaction-initiating species; and

(b) irradiating the multiphoton-activatable, photoreactive composition with light sufficient to cause absorption of at least two photons, thereby inducing at least one acid- or radical-initiated chemical reaction where the composition is exposed to the light.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 16 OF 33 USPATFULL on STN
AB A photoreactive composition comprises (a) at least one reactive species that is capable of undergoing an acid- or radical-initiated chemical reaction; and (b) a photoinitiator system comprising photochemically-effective amounts of (1) at least one type of semiconductor nanoparticle quantum dot that has at least one electronic excited state that is accessible by absorption of two or more photons, and (2) a composition, different from said reactive species, that is capable of interacting with the excited state of the semiconductor nanoparticle quantum dot to form at least one reaction-initiating species.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 17 OF 33 USPATFULL on STN
AB One aspect of the present invention relates to ionic liquids comprising a pendant Bronsted-acidic group, e.g., a sulfonic acid group. Another aspect of the present invention relates to the use of an ionic liquid comprising a pendant Bronsted-acidic group to catalyze a Bronsted-acid-catalyzed chemical reaction. A third aspect of the present invention relates to ionic liquids comprising a pendant nucleophilic group, e.g., an amine. Still another aspect of the present invention relates to the use of an ionic liquid comprising a pendant nucleophilic group to catalyze a nucleophile-assisted chemical reaction. A fifth aspect of the present invention relates to the use of an ionic liquid comprising a pendant nucleophilic group to remove a gaseous impurity, e.g., carbon dioxide, from a gas, e.g., sour natural gas.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 18 OF 33 USPATFULL on STN
AB There is provided a novel fluorine-containing polymer having an acid-reactive group which has a high transparency against energy rays (radioactive rays) in a vacuum ultraviolet region (157 nm), and further there are provided a material for fluorine-containing base polymer prepared from the polymer and suitable for a photoresist and a chemically amplifying type resist composition obtained therefrom.

The polymer has a number average molecular weight of from 1,000 to 1,000,000 and represented by the formula:

-(M1)-(M2)-(A)-,

wherein M1 is a structural unit having an acid-labile or acid-degradable functional group, M2 is a structural unit of fluorine-containing acryl ester, A is a structural unit derived from other copolymerizable monomer, the percent by mole ratio M1/M2 is 1 to 99/99 to 1 and the polymer comprises from 1 to 99% by mole of the structural unit M1, from 1 to 99% by mole of the structural unit M2 and from 0 to 98% by mole of the structural unit A1. The material for fluorine-containing base polymer comprises a fluorine-containing polymer having an acid-reactive group such as the above-mentioned polymer and is suitable for a photoresist, and the chemically amplifying type resist composition is obtained from those polymer and material.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 19 OF 33 USPATFULL on STN
AB A multiphoton-activatable, photoreactive composition comprises: (a) at least one reactive species that is capable of undergoing an acid- or radical-initiated chemical reaction; (b) a photochemically-effective amount of a multiphoton photosensitizer comprising at least one multiphoton up-converting inorganic phosphor; and (c) a photochemically-effective amount of a one-photon photoinitiator system that is capable of being photosensitized by the multiphoton photosensitizer.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 20 OF 33 USPATFULL on STN

AB The application discloses novel synthetic compounds, modeled after unique toxins extracted from the marine invertebrate Diazona angulata useful in the treatment abnormal cell mitosis. The application also discloses novel methods for synthesis of these compounds and methods of using these compounds.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 21 OF 33 USPATFULL on STN

AB A process of forming a resist image in a microelectronic substrate comprises the steps of contacting the substrate with a composition first comprising carbon dioxide and a component selected from the group consisting of at least one polymeric precursor, at least one monomer, at least one polymeric material, and mixtures thereof to deposit the component on the substrate and form a coating thereon; then imagewise exposing the coating to radiation such that exposed and unexposed coating portions are formed; then subjecting the coating to a second composition comprising carbon dioxide having such that either one of the exposed or the unexposed coating portions are removed from the substrate and the other coating portion is developed and remains on the coating to form an image thereon.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 22 OF 33 USPATFULL on STN

AB The present invention provides a negative photosensitive resin composition comprising (A) a photocurable resin having a photosensitive group or groups crosslinkable by light irradiation, (B) a photoacid generator and (C) a photosensitizer which is a benzopyran condensed ring compound capable of increasing photosensitivity to visible light with a wavelength of 480 nm or more,

a negative photosensitive dry film prepared by applying the photosensitive resin composition to a surface of support film, followed by drying, to form a photosensitive resin layer, and

a method of forming a pattern using the resin composition or the dry film.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 23 OF 33 USPATFULL on STN

AB Radiation-sensitive compositions comprising

(a1) a cationically or acid-catalytically polymerisable or crosslinkable compound or

(a2) a compound that increases its solubility in a developer under the action of acid; and

(b) at least one diaryliodonium salt of formula I ##STR1##

X is branched C.sub.3 -C.sub.20 alkyl or C.sub.3 -C.sub.8 cycloalkyl;

X.sub.1 is hydrogen, linear C.sub.1 -C.sub.20 alkyl, branched C.sub.3 -C.sub.20 alkyl or C.sub.3 -C.sub.8 cycloalkyl; with the proviso that the sum of the carbon atoms in X and X.sub.1 is at least 4;

Y is linear C.sub.1 -C.sub.10 alkyl, branched C.sub.3 -C.sub.10 alkyl or C.sub.3 -C.sub.8 cycloalkyl;

A.sup.- is a non-nucleophilic anion, selected from the group (BF.sub.4).sup.-, (SbF.sub.6).sup.-, (PF.sub.6).sup.-, (B(C.sub.6 F.sub.5)).sub.4.sup.-, C.sub.1 -C.sub.20 alkylsulfonate, C.sub.2 -C.sub.20 haloalkylsulfonate, unsubstituted C.sub.6 -C.sub.10 arylsulfonate, camphorsulfonate, and C.sub.6 -C.sub.10 arylsulfonate substituted by halogen, NO.sub.2, C.sub.1 -C.sub.12 alkyl, C.sub.1 -C.sub.12 halo-alkyl, C.sub.1 -C.sub.12 alkoxy or by COOR.sub.1 ; and

R.sub.1 is C.sub.1 -C.sub.20 alkyl, phenyl, benzyl; or phenyl mono- or poly-substituted by C.sub.1 -C.sub.12 alkyl, C.sub.1 -C.sub.12 alkoxy or by halogen;

with the proviso that the two phenyl rings on the iodine atom are not identically substituted.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 24 OF 33 USPATFULL on STN

AB A negative type photosensitive resin composition is herein disclosed which is used under the irradiation circumstance of a safelight having a maximum wavelength within the range of 500 to 620 nm and a large spectral luminous efficiency; the composition being a liquid or a solid resin composition containing a photocurable resin, a photoreaction initiator and if necessary, a photosensitizing dye; an absorbancy of an unexposed film formed from this composition being 0.5 or less within the range of the maximum wavelength ±30 nm selected from the range of the maximum wavelength of the safelight. By the use of this negative type photosensitive resin composition, it is possible to form a resist pattern which is excellent in safe operativity, operational efficiency, the quality stability of products, and the like.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 25 OF 33 USPATFULL on STN

AB A visible light curable resin composition containing a photocurable resin, a photoreaction initiator and a photosensitizer having the formula (1). The composition has a very high sensitivity to a general-purpose visible light laser, so that a high-speed scanning exposure is possible by the laser, and an extremely fine high resolution can be obtained. In addition, the composition can be used for coating or printing under safelight irradiating conditions and under bright circumstantial conditions without any thickening of the composition, and hence the composition can exert excellent noticeable effects in points of safe operativity, operational efficiency and the stability of products. Formula (1) is as follows: ##STR1## wherein rings X.sub.1 and X.sub.2 are each an optionally substituted pyrrole ring; Y is H, CN, optionally substituted alkyl, aralkyl, aryl, heteroaryl or alkenyl group; and Z.sub.1 and Z.sub.2 are halogen, optionally substituted alkyl, alkoxy, alkylthio, aralkyl, aralkyloxy, aryl, aryloxy, arylthio, heteroaryl, heteroaryloxy or heteroarylthio group, provided that at least one of substituents on the pyrrole rings X.sub.1 and X.sub.2, groups Z.sub.1 and Z.sub.2 is the alkoxy, aralkyloxy or aryloxy group.

L7 ANSWER 26 OF 33 USPATFULL on STN

AB 2-Aryl-1,3-cyclopentanedione enol ester compounds exhibit outstanding acaricidal and herbicidal activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 27 OF 33 USPATFULL on STN
AB 2-Aryl-1,3-cyclopentanedione enol ester compounds exhibit outstanding acaricidal and herbicidal activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 28 OF 33 USPATFULL on STN
AB Non-ortho substituted 2-aryl-1,3-cycloalkanedione enol ester compounds exhibit outstanding acaricidal and herbicidal activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 29 OF 33 USPATFULL on STN
AB Enol derivatives of 2-aryl-1,3-cycloalkanedione compounds exhibit outstanding herbicidal and acarcidal activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 30 OF 33 USPATFULL on STN
AB 2-Aryl-1,3-cyclopentanedione compounds and their alkali metal and ammonium salts exhibit outstanding herbicidal and acaricidal activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 31 OF 33 USPATFULL on STN
AB 2-Aryl-1,3-cyclopentanedione compounds and their alkali metal and ammonium salts exhibit outstanding herbicidal and acaricidal activity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L7 ANSWER 32 OF 33 DISSABS COPYRIGHT (C) 2009 ProQuest Information and Learning Company; All Rights Reserved on STN
AB Bridged ring cores possessing quaternary carbon centers adjacent to a bridged ketone constitute challenging structures in synthesis. Therefore, this thesis explores the development of the first Prins-pinacol synthesis of cis-fused bicyclo[4,n,1]alkanones. The reaction conditions were optimized for the rearrangement of bicyclo[4.4.0]decanes and the effect of different diol protecting groups was explored, as well as the effect of substitution at the C4 and the C5 position. The rearrangement of bicyclo[5.4.0]undecane and bicyclo[5.3.0]decanes was also investigated in order to achieve the formation of bicyclic ketones with various ring sizes. Finally, the Prins-pinacol rearrangement was coupled with an ionic Diels-Alder reaction in order to achieve the rapid synthesis of highly functionalized polycyclic bridgehead ketones.

L7 ANSWER 33 OF 33 DISSABS COPYRIGHT (C) 2009 ProQuest Information and Learning Company; All Rights Reserved on STN
AB As a stereochemically complementary method to the dioxanone-to-dihydropyran route developed in the Burke laboratories, highly stereoselective syntheses of anti 2,3-disubstituted tetrahydropyrans were accomplished utilizing intramolecular radical cyclization, featuring captodative stabilization and late, tight transition states.

In an extended study, 2,3-disubstituted tetrahydrofurans were synthesized using the same technique as in the tetrahydropyran syntheses, where anti diastereomers were obtained as the dominant product. In addition, anionic cyclizations of appropriate acyclic precursors resulted in the highly stereoselective syntheses of anti 2,3-disubstituted tetrahydrofurans.

The syntheses of tetrahydrofurans were directly applied to the stereo-divergent formal total syntheses of two natural mold metabolites, avenaciolide and isoavenaciolide. The salient features involved in the synthesis included the intramolecular Pummerer rearrangement and C-allylation.

The last issue in this dissertation is focused on the synthesis of the C(1)-C(14) subunit of halichondrin B, a tubulin-based antimitotic anticancer agent. Included in the synthesis are a pinacol rearrangement, intramolecular Michael addition, and a one-pot multistep conversion leading to the formation of the lipophilic polycyclic ketal, the C(8)-C(14) substructure of halichondrin B.

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L3          16 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 08:42:05 ON 21 JUN 2009
L4           5 S L3

     FILE 'CAPLUS, USPATFULL, DISSABS' ENTERED AT 08:47:32 ON 21 JUN 2009
L5         814 S PINACOL REARRANGEMENT
L6        3418 S L5 (L) POLYCYCLIC OR MULTICYCLIC
L7          33 S PINACOL REARRANGEMENT (L) POLYCYCLIC
L8          33 DUP REM L7 (0 DUPLICATES REMOVED)
L9         240 S PINACOL REARRANGEMENT/TI
L10          2 S L9 AND L7
L11        407 S PINACOL REARRANGEMENT/AB
L12        110 S L11 AND L9
L13          5 S L11 AND L7
L14          4 S L13 NOT L10

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L6        3418 SEA SPE=ON  ABB=ON  PLU=ON  L5 (L) POLYCYCLIC OR MULTICYCLIC
L7          33 SEA SPE=ON  ABB=ON  PLU=ON  PINACOL REARRANGEMENT (L) POLYCYCLI
               C
L8          33 DUP REM L7 (0 DUPLICATES REMOVED)
L9         240 SEA SPE=ON  ABB=ON  PLU=ON  PINACOL REARRANGEMENT/TI
L10          2 SEA SPE=ON  ABB=ON  PLU=ON  L9 AND L7
               D 1-2 IBIB ABS
L11        407 SEA SPE=ON  ABB=ON  PLU=ON  PINACOL REARRANGEMENT/AB
L12        110 SEA SPE=ON  ABB=ON  PLU=ON  L11 AND L9
L13          5 SEA SPE=ON  ABB=ON  PLU=ON  L11 AND L7
L14          4 SEA SPE=ON  ABB=ON  PLU=ON  L13 NOT L10
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L16          0 SEA SPE=ON  ABB=ON  PLU=ON  L7 NOT L10

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                                                   ENTRY    SESSION
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                 information
 NEWS  6  APR 26 USPATFULL and USPAT2 enhanced with patent
                 assignment/reassignment information
 NEWS  7  APR 28 CAS patent authority coverage expanded
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 NEWS  9  APR 28 Limits doubled for structure searching in CAS
                 REGISTRY
 NEWS 10  MAY 08 STN Express, Version 8.4, now available
 NEWS 11  MAY 11 STN on the Web enhanced
 NEWS 12  MAY 11 BEILSTEIN substance information now available on
                 STN Easy
 NEWS 13  MAY 14 DGENE, PCTGEN and USGENE enhanced with increased
                 limits for exact sequence match searches and
                 introduction of free HIT display format
 NEWS 14  MAY 15 INPADOCDB and INPAFAMDB enhanced with Chinese legal
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 NEWS 15  MAY 28 CAS databases on STN enhanced with NANO super role in
                 records back to 1992
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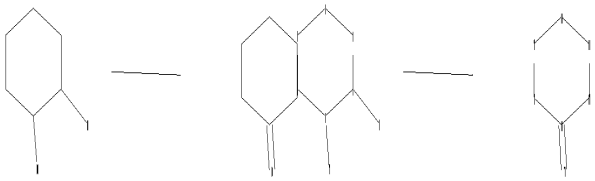

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ring nodes :
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ring bonds :
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exact bonds :
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Match level :
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13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS
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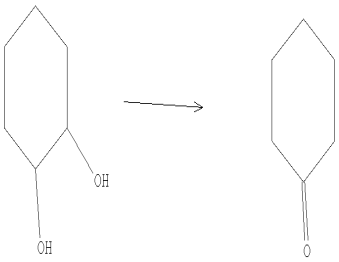

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MULTIPLE ROLE QUERIES ARE NOT ALLOWED IN A NON-REACTION FILE

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SEARCH TIME: 00.00.06

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
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PROJECTED ANSWERS:             515 TO     1327

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=> d 1-11 ibib hit


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AUTHOR(S):              Tamiya, Minoru; Ohmori, Ken; Kitamura, Mitsuru; Kato,
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CORPORATE SOURCE:       Department of Chemistry, Tokyo Institute of
                        Technology, 2-12-1 O-okayama, Meguro-ku Tokyo,
                        152-8551, Japan
SOURCE:                 Chemistry--A European Journal (2007), 13(35),
                        9791-9823
                        CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER:              Wiley-VCH Verlag GmbH & Co. KGaA
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                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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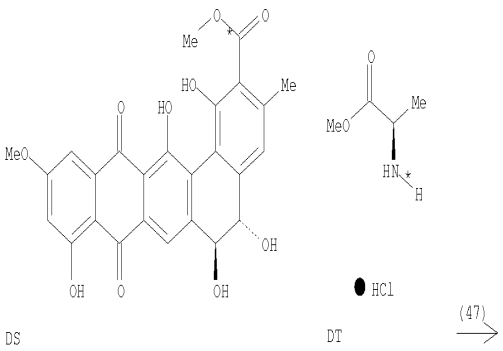
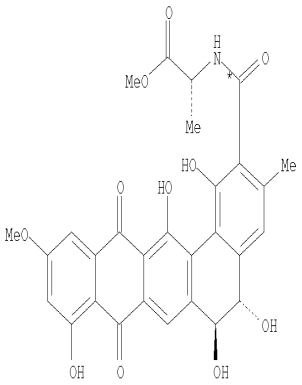
RX(47) OF 977 ...DS + DT ===> DU...



DS DT



DU
YIELD 63%

RX(47) RCT DS 236752-00-4, DT 14316-06-4

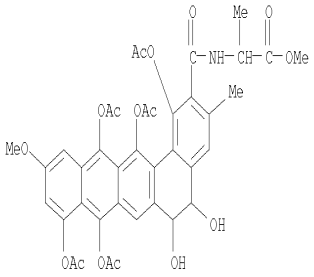
STAGE(1)
RGT DV 56602-33-6 BOP reagent, O 121-44-8 Et3N
CON 1.5 hours, room temperature

STAGE(2)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water

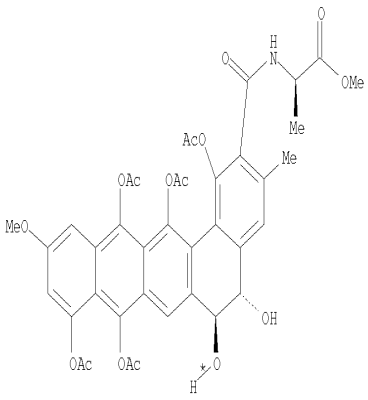
PRO DU 116249-67-3

RX(168) OF 977 COMPOSED OF RX(50), RX(51)

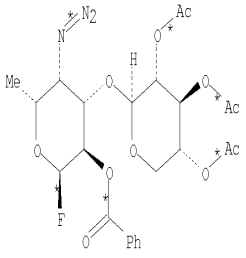
RX(168) 2 EA + 2 EB ===> EG



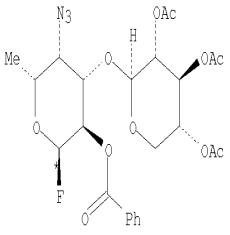
EA



EA



EB



EB

2
STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(50)

STAGE(1)
RGT EE 12116-66-4 Hafnocene dichloride, EF 7783-93-9 AgClO4
SOL 75-09-2 CH2Cl2
CON 10 minutes, room temperature

STAGE(2)
RCT EA 149726-04-5, EB 303153-45-9
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -12 deg C
SUBSTAGE(3) 25 minutes, -12 deg C

STAGE(3)
RGT AC 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO EC 1007851-87-7, ED 1007851-89-9
NTE molecular sieves used, regioselective

RX(51) RCT EC 1007851-87-7

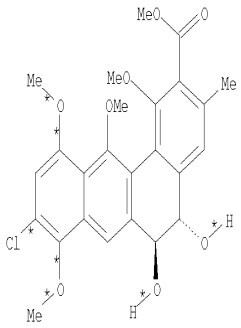
STAGE(1)
RGT BV 7647-01-0 HCl, EH 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 6 hours, room temperature

STAGE(2)
RGT CQ 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 2 hours, room temperature

STAGE(3)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water, 67-56-1 MeOH
CON pH 3.5

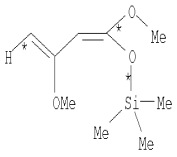
PRO EG 116299-57-1

RX(332) OF 977 COMPOSED OF RX(42), RX(43), RX(44)
RX(332) DL + 2 AM + AX ===> DP



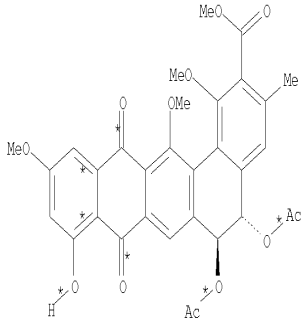
DL

2 AM



AX

3
STEPS



DP
YIELD 90%

RX(42) RCT DL 236751-93-2, AM 108-24-7

STAGE(1)
CAT 1122-58-3 4-DMAP
SOL 110-86-1 Pyridine
CON 20 minutes, room temperature

STAGE(2)
RGT K 7732-18-5 Water

PRO DN 1007851-75-3

RX(43) RCT DN 1007851-75-3

STAGE(1)
RGT AV 10139-51-2 (NH4)2Ce(NO3)6
SOL 7732-18-5 Water, 75-05-8 MeCN
CON 10 minutes, 0 deg C

STAGE(2)
RGT K 7732-18-5 Water

PRO DO 236751-96-5

RX(44) RCT AX 106875-55-2, DO 236751-96-5

STAGE(1)
SOL 109-99-9 THF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 2 hours, room temperature

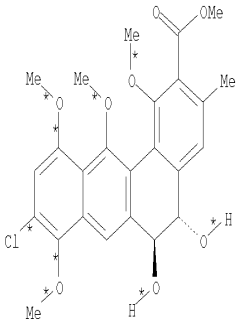
STAGE(2)
RGT BD 7631-86-9 SiO2
CON SUBSTAGE(1) pH 6
SUBSTAGE(2) 12 hours, room temperature

STAGE(3)
RGT E 584-08-7 K2CO3
SOL 109-99-9 THF, 75-09-2 CH2Cl2
CON 2.5 hours, room temperature

STAGE(4)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water

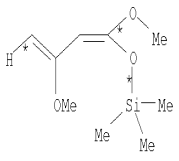
PRO DP 236751-98-7
NTE Diels-Alder reaction, regioselective

RX(335) OF 977 COMPOSED OF RX(42), RX(43), RX(44), RX(45)
RX(335) DL + 2 AM + AX ===> DQ



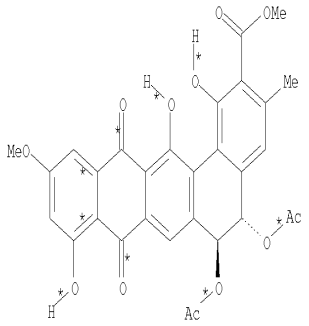
DL

2 AM



AX

4
STEPS



DQ
YIELD 99%

RX(42) RCT DL 236751-93-2, AM 108-24-7

STAGE(1)
CAT 1122-58-3 4-DMAP
SOL 110-86-1 Pyridine
CON 20 minutes, room temperature

STAGE(2)
RGT K 7732-18-5 Water

PRO DN 1007851-75-3

RX(43) RCT DN 1007851-75-3

STAGE(1)
RGT AV 10139-51-2 (NH4)2Ce(NO3)6
SOL 7732-18-5 Water, 75-05-8 MeCN
CON 10 minutes, 0 deg C

STAGE(2)
RGT K 7732-18-5 Water

PRO DO 236751-96-5

RX(44) RCT AX 106875-55-2, DO 236751-96-5

STAGE(1)
SOL 109-99-9 THF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 2 hours, room temperature

STAGE(2)
RGT BD 7631-86-9 SiO2
CON SUBSTAGE(1) pH 6
SUBSTAGE(2) 12 hours, room temperature

STAGE(3)
RGT E 584-08-7 K2CO3
SOL 109-99-9 THF, 75-09-2 CH2Cl2
CON 2.5 hours, room temperature

STAGE(4)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water

PRO DP 236751-98-7
NTE Diels-Alder reaction, regioselective

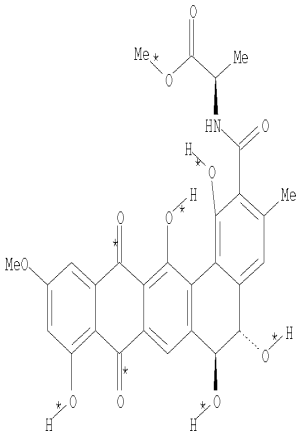
RX(45) RCT DP 236751-98-7

STAGE(1)
RGT DR 10294-34-5 BCl3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON 30 minutes, -10 deg C

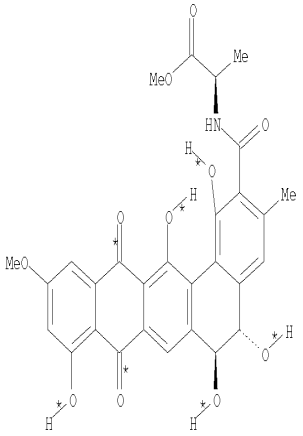
STAGE(2)
RGT AC 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DQ 236751-99-8

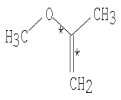
RX(347) OF 977 COMPOSED OF RX(48), RX(49), RX(50), RX(51)
RX(347) 2 DU + DW + 10 AM + 2 EB ===> EG



DU

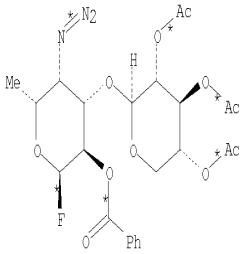


DU

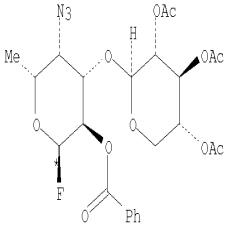


DW

10 AM



EB



EB

4

STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(48) RCT DU 116249-67-3, DW 116-11-0

STAGE(1)
CAT 6192-52-5 p-MeC6H4SO3H.H2O
SOL 68-12-2 DMF
CON 18 hours, room temperature

STAGE(2)
RGT K 7732-18-5 Water

STAGE(3)
RCT AM 108-24-7
RGT DY 7440-66-6 Zn
SOL 110-86-1 Pyridine
CON 10 hours, room temperature

STAGE(4)
RGT AD 67-56-1 MeOH

PRO DX 1007851-83-3
NTE regioselective

RX(49) RCT DX 1007851-83-3

STAGE(1)
RGT DZ 6192-52-5 p-MeC6H4SO3H.H2O
SOL 7732-18-5 Water, 75-05-8 MeCN
CON 2 hours, room temperature

STAGE(2)
RGT K 7732-18-5 Water

PRO EA 149726-04-5
NTE chemoselective

RX(50)

STAGE(1)
RGT EE 12116-66-4 Hafnocene dichloride, EF 7783-93-9 AgClO4
SOL 75-09-2 CH2Cl2
CON 10 minutes, room temperature

STAGE(2)
RCT EA 149726-04-5, EB 303153-45-9
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -12 deg C
SUBSTAGE(3) 25 minutes, -12 deg C

STAGE(3)
RGT AC 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO EC 1007851-87-7, ED 1007851-89-9
NTE molecular sieves used, regioselective

RX(51) RCT EC 1007851-87-7

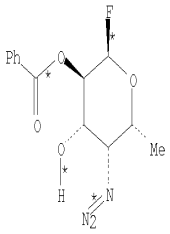
STAGE(1)
RGT BV 7647-01-0 HCl, EH 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 6 hours, room temperature

STAGE(2)
RGT CQ 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 2 hours, room temperature

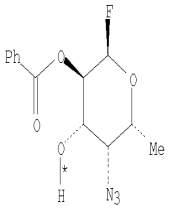
STAGE(3)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water, 67-56-1 MeOH
CON pH 3.5

PRO EG 116299-57-1

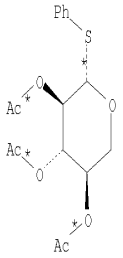
RX(473) OF 977 COMPOSED OF RX(105), RX(50), RX(51)
RX(473) 3 HV + 3 HY + 2 EA ===> EG



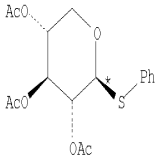
HV



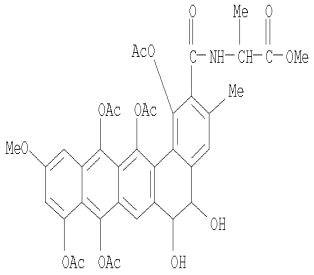
2 HV



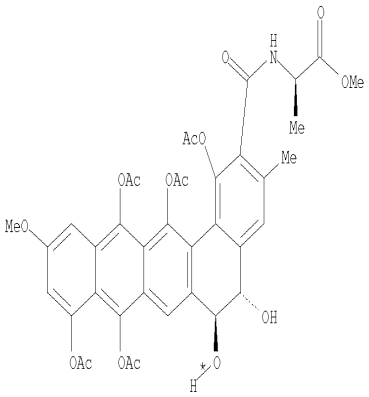
HY



2 HY



EA



EA

3
STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(105) RCT HV 303153-48-2, HY 62774-34-9

STAGE(1)
RGT IA 516-12-1 Iodosuccinimide
CAT 1493-13-6 F3CSO2H
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -40 deg C
SUBSTAGE(2) 10 minutes, -78 deg C
SUBSTAGE(3) 2 hours, -40 deg C

STAGE(2)
RGT AC 144-55-8 NaHCO3, BQ 7775-14-6 Na2(S2O4)
SOL 7732-18-5 Water

PRO EB 303153-45-9, HZ 1007854-77-4
NTE molecular sieves used, stereoselective

RX(50)

STAGE(1)
RGT EE 12116-66-4 Hafnocene dichloride, EF 7783-93-9 AgClO4
SOL 75-09-2 CH2Cl2
CON 10 minutes, room temperature

STAGE(2)
RCT EA 149726-04-5, EB 303153-45-9
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -12 deg C
SUBSTAGE(3) 25 minutes, -12 deg C

STAGE(3)
RGT AC 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO EC 1007851-87-7, ED 1007851-89-9
NTE molecular sieves used, regioselective

RX(51) RCT EC 1007851-87-7

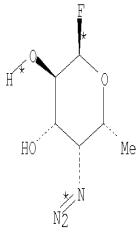
STAGE(1)
RGT BV 7647-01-0 HCl, EH 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 6 hours, room temperature

STAGE(2)
RGT CQ 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 2 hours, room temperature

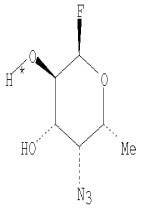
STAGE(3)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water, 67-56-1 MeOH
CON pH 3.5

PRO EG 116299-57-1

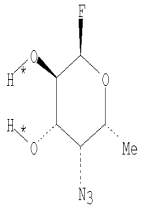
RX(477) OF 977 COMPOSED OF RX(104), RX(105), RX(50), RX(51)
RX(477) 4 HS + 5 HU + 3 HY + 2 EA ===> EG



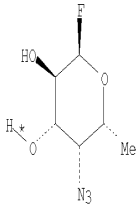
HS



HS

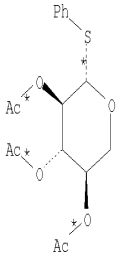


HS

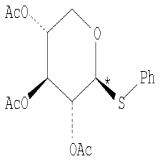


HS

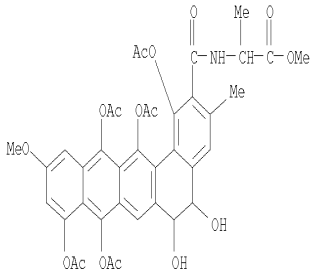
5 HU



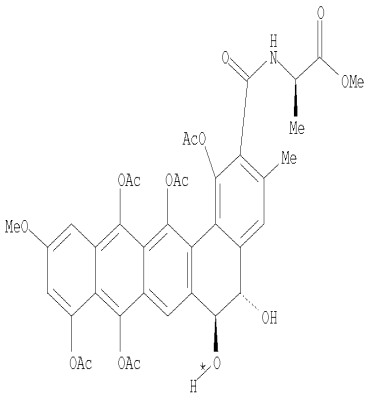
HY



2 HY



EA



EA

4 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(104) RCT HS 303153-47-1, HU 98-88-4

STAGE(1)
SOL 75-09-2 CH2Cl2, 110-86-1 Pyridine
CON 15 hours, 0 deg C

STAGE(2)
RGT BT 109-55-7 Me2N(CH2)3NH2
CON 5 minutes, 0 deg C

PRO HV 303153-48-2, HW 1007854-68-3, HX 1007854-71-8

RX(105) RCT HV 303153-48-2, HY 62774-34-9

STAGE(1)
RGT IA 516-12-1 Iodosuccinimide
CAT 1493-13-6 F3CSO2H
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -40 deg C
SUBSTAGE(2) 10 minutes, -78 deg C
SUBSTAGE(3) 2 hours, -40 deg C

STAGE(2)
RGT AC 144-55-8 NaHCO3, BQ 7775-14-6 Na2(S2O4)
SOL 7732-18-5 Water

PRO EB 303153-45-9, HZ 1007854-77-4
NTE molecular sieves used, stereoselective

RX(50)

STAGE(1)
RGT EE 12116-66-4 Hafnocene dichloride, EF 7783-93-9 AgClO4
SOL 75-09-2 CH2Cl2
CON 10 minutes, room temperature

STAGE(2)
RCT EA 149726-04-5, EB 303153-45-9
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -12 deg C
SUBSTAGE(3) 25 minutes, -12 deg C

STAGE(3)
RGT AC 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO EC 1007851-87-7, ED 1007851-89-9
NTE molecular sieves used, regioselective

RX(51) RCT EC 1007851-87-7

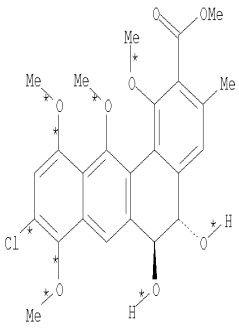
STAGE(1)
RGT BV 7647-01-0 HCl, EH 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 6 hours, room temperature

STAGE(2)
RGT CQ 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 2 hours, room temperature

STAGE(3)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water, 67-56-1 MeOH
CON pH 3.5

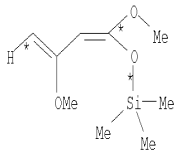
PRO EG 116299-57-1

RX(705) OF 977 COMPOSED OF RX(42), RX(43), RX(44), RX(45), RX(46)
RX(705) DL + 2 AM + AX ===> DS



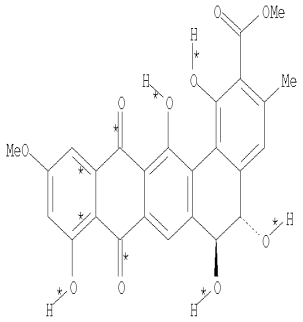
DL

2 AM



AX

5
STEPS



DS

RX(42) RCT DL 236751-93-2, AM 108-24-7

STAGE(1)
CAT 1122-58-3 4-DMAP
SOL 110-86-1 Pyridine
CON 20 minutes, room temperature

STAGE(2)
RGT K 7732-18-5 Water

PRO DN 1007851-75-3

RX(43) RCT DN 1007851-75-3

STAGE(1)
RGT AV 10139-51-2 (NH4)2Ce(NO3)6
SOL 7732-18-5 Water, 75-05-8 MeCN
CON 10 minutes, 0 deg C

STAGE(2)

RGT K 7732-18-5 Water

PRO DO 236751-96-5

RX(44) RCT AX 106875-55-2, DO 236751-96-5

STAGE(1)
SOL 109-99-9 THF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 2 hours, room temperature

STAGE(2)
RGT BD 7631-86-9 SiO2
CON SUBSTAGE(1) pH 6
SUBSTAGE(2) 12 hours, room temperature

STAGE(3)
RGT E 584-08-7 K2CO3
SOL 109-99-9 THF, 75-09-2 CH2Cl2
CON 2.5 hours, room temperature

STAGE(4)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water

PRO DP 236751-98-7
NTE Diels-Alder reaction, regioselective

RX(45) RCT DP 236751-98-7

STAGE(1)
RGT DR 10294-34-5 BCl3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON 30 minutes, -10 deg C

STAGE(2)
RGT AC 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DQ 236751-99-8

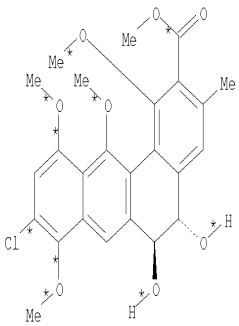
RX(46) RCT DQ 236751-99-8

STAGE(1)
RGT CQ 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) 2.5 hours, 70 deg C
SUBSTAGE(2) 70 deg C -> room temperature

STAGE(2)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water
CON acidify

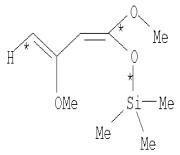
PRO DS 236752-00-4

RX(710) OF 977 COMPOSED OF RX(42), RX(43), RX(44), RX(45), RX(46), RX(47)
RX(710) DL + 2 AM + AX + DT ===> DU

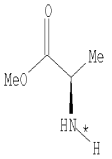


DL

2 AM



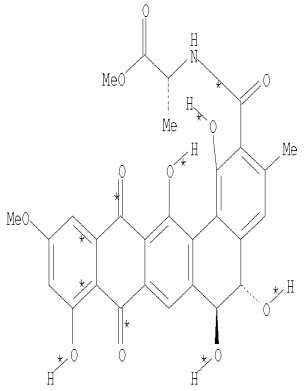
AX



DT

HCl

6
STEPS



DU
YIELD 63%

RX(42) RCT DL 236751-93-2, AM 108-24-7

STAGE(1)
CAT 1122-58-3 4-DMAP
SOL 110-86-1 Pyridine
CON 20 minutes, room temperature

STAGE(2)
RGT K 7732-18-5 Water

PRO DN 1007851-75-3

RX(43) RCT DN 1007851-75-3

STAGE(1)
RGT AV 10139-51-2 (NH4)2Ce(NO3)6

SOL 7732-18-5 Water, 75-05-8 MeCN
CON 10 minutes, 0 deg C

STAGE(2)
RGT K 7732-18-5 Water

PRO DO 236751-96-5

RX(44) RCT AX 106875-55-2, DO 236751-96-5

STAGE(1)
SOL 109-99-9 THF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 2 hours, room temperature

STAGE(2)
RGT BD 7631-86-9 SiO2
CON SUBSTAGE(1) pH 6
SUBSTAGE(2) 12 hours, room temperature

STAGE(3)
RGT E 584-08-7 K2CO3
SOL 109-99-9 THF, 75-09-2 CH2Cl2
CON 2.5 hours, room temperature

STAGE(4)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water

PRO DP 236751-98-7
NTE Diels-Alder reaction, regioselective

RX(45) RCT DP 236751-98-7

STAGE(1)
RGT DR 10294-34-5 BCl3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON 30 minutes, -10 deg C

STAGE(2)
RGT AC 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DQ 236751-99-8

RX(46) RCT DQ 236751-99-8

STAGE(1)
RGT CQ 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) 2.5 hours, 70 deg C
SUBSTAGE(2) 70 deg C -> room temperature

STAGE(2)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water
CON acidify

PRO DS 236752-00-4

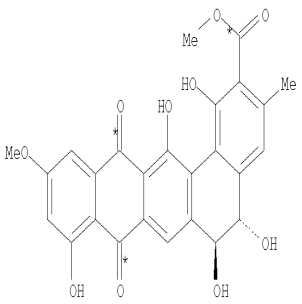
RX(47) RCT DS 236752-00-4, DT 14316-06-4

STAGE(1)
RGT DV 56602-33-6 BOP reagent, O 121-44-8 Et3N
CON 1.5 hours, room temperature

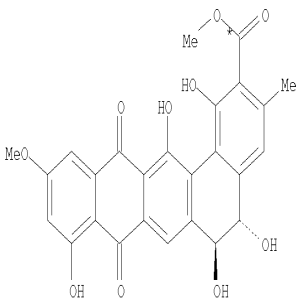
STAGE(2)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water

PRO DU 116249-67-3

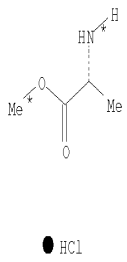
RX(725) OF 977 COMPOSED OF RX(47), RX(48), RX(49), RX(50), RX(51)
RX(725) 2 DS + 2 DT + DW + 10 AM + 2 EB ===> EG



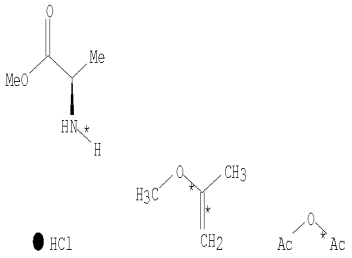
DS



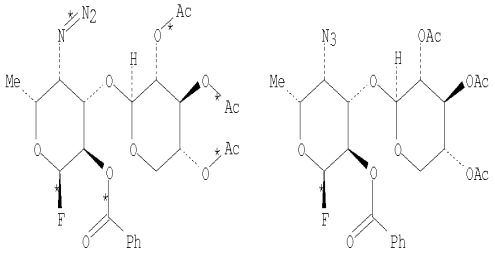
DS



DT



DT DW 10 AM



EB EB

5
STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(47) RCT DS 236752-00-4, DT 14316-06-4

STAGE(1)
RGT DV 56602-33-6 BOP reagent, O 121-44-8 Et3N
CON 1.5 hours, room temperature

STAGE(2)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water

PRO DU 116249-67-3

RX(48) RCT DU 116249-67-3, DW 116-11-0

STAGE(1)
CAT 6192-52-5 p-MeC6H4SO3H.H20
SOL 68-12-2 DMF
CON 18 hours, room temperature

STAGE(2)
RGT K 7732-18-5 Water

STAGE(3)
RCT AM 108-24-7
RGT DY 7440-66-6 Zn
SOL 110-86-1 Pyridine
CON 10 hours, room temperature

STAGE(4)
RGT AD 67-56-1 MeOH

PRO DX 1007851-83-3
NTE regioselective

RX(49) RCT DX 1007851-83-3

STAGE(1)
RGT DZ 6192-52-5 p-MeC6H4SO3H.H20
SOL 7732-18-5 Water, 75-05-8 MeCN
CON 2 hours, room temperature

STAGE(2)
RGT K 7732-18-5 Water

PRO EA 149726-04-5
NTE chemoselective

RX(50)

STAGE(1)
RGT EE 12116-66-4 Hafnocene dichloride, EF 7783-93-9 AgClO4
SOL 75-09-2 CH2Cl2
CON 10 minutes, room temperature

STAGE(2)
RCT EA 149726-04-5, EB 303153-45-9
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -12 deg C
SUBSTAGE(3) 25 minutes, -12 deg C

STAGE(3)
RGT AC 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO EC 1007851-87-7, ED 1007851-89-9
NTE molecular sieves used, regioselective

RX(51) RCT EC 1007851-87-7

STAGE(1)
RGT BV 7647-01-0 HCl, EH 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 6 hours, room temperature

STAGE(2)

RGT CQ 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 2 hours, room temperature

STAGE(3)
RGT BV 7647-01-0 HCl
SOL 7732-18-5 Water, 67-56-1 MeOH
CON pH 3.5

PRO EG 116299-57-1

AB A general approach to the regio- and stereoselective total synthesis of the benanomicin-pradimicin antibiotics (BpAs) is described. Construction of the aglycon has been achieved by (1) the diastereoselective ring-opening of biaryl lactone I by using (R)-valinol as a chiral nucleophile and (2) the stereocontrolled semi-pinacol cyclization of the aldehyde acetal II by using SmI2 in the presence of BF3-OEt2 and a proton source to afford the ABCD tetracyclic monoprotected diol III (R = CH2Ph). This strategy enabled us to control the two stereogenic sites in the B ring (C-5 and C-6) and the regioselective introduction of the carbohydrate moiety. The ABCD tetracycle could serve as an ideal platform for the divergent access to various BpAs. The amino acid (D-alanine) was introduced onto the ABCD tetracycle. Glycosylation was promoted by the combination of Cp2HfCl2 and AgOTf (1:2 ratio). Construction of the E ring followed by deprotection completed the first total synthesis of benanomicin A, benanomicin B, and pradimicin A. The route is flexible enough to allow the synthesis of other congeners differing in their amino acid and carbohydrate moieties.

ST benanomicin pradimicin antibiotic synthesis diastereoselective ring opening pinacol cyclization; regioselective stereoselective synthesis benanomicin pradimicin antibiotic

IT Glycosylation
Stereoselective synthesis
(regio- and stereoselective total synthesis of benanomicin-pradimicin antibiotics via diastereoselective ring-opening, semi-pinacol cyclization, and glycosylation)

IT Cyclization
(semi-pinacol; regio- and stereoselective total synthesis of benanomicin-pradimicin antibiotics via diastereoselective ring-opening, semi-pinacol cyclization, and glycosylation)

IT Ring opening
(stereoselective; regio- and stereoselective total synthesis of benanomicin-pradimicin antibiotics via diastereoselective ring-opening, semi-pinacol cyclization, and glycosylation)

IT 141020-08-8P 152039-22-0P 1007851-47-9P 1007851-89-9P
1007852-02-9P 1007852-13-2P 1007852-18-7P 1007852-66-5P
1007852-72-3P 1007852-99-4P 1007853-09-9P 1007853-15-7P
1007854-27-4P 1007854-39-8P 1007854-68-3P 1007854-71-8P
1007855-05-1P 1007855-09-5P 1007855-12-0P 1007855-15-3P
1007855-17-5P 1007855-19-7P 1007855-23-3P 1009073-16-8P
RL: BYP (Byproduct); PREP (Preparation)
(regio- and stereoselective total synthesis of benanomicin-pradimicin antibiotics via diastereoselective ring-opening, semi-pinacol cyclization, and glycosylation)

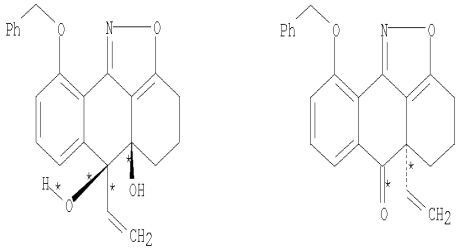
IT 59-23-4, D-Galactose, reactions 72-18-4, L-Valine, reactions 100-52-7, Benzaldehyde, reactions 108-95-2, Phenol, reactions 492-41-1
2749-11-3 3182-95-4 3187-58-4, Methyl 2,4-dihydroxy-6-methylbenzoate
4276-09-9 14316-06-4, D-Alanine methyl ester hydrochloride 17431-03-7
18113-03-6, 2-Chloro-4-methoxyphenol 29868-42-6 39637-74-6,
(-)-Camphanic chloride 62774-34-9 64715-88-4 77924-28-8
106875-55-2 112245-13-3 152039-10-6 863423-82-9 1007852-86-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(regio- and stereoselective total synthesis of benanomicin-pradimicin antibiotics via diastereoselective ring-opening, semi-pinacol cyclization, and glycosylation)

IT 93-02-7P, 2,5-Dimethoxybenzaldehyde 1824-94-8P, Methyl β-D-Galactopyranoside 10368-78-2P 22435-34-3P 25932-95-0P
42214-04-0P 43139-92-0P 64552-06-3P 116249-67-3P 141116-05-4P
147589-45-5P 149726-04-5P 152039-03-7P 152039-05-9P 157188-14-2P
236751-38-5P 236751-40-9P 236751-42-1P 236751-45-4P 236751-48-7P
236751-54-5P 236751-58-9P 236751-71-6P 236751-74-9P 236751-78-3P
236751-82-9P 236751-86-3P 236751-90-9P 236751-93-2P 236751-96-5P
236751-98-7P 236751-99-8P 236752-00-4P 236755-03-6P 236755-05-8P
303153-45-9P 303153-46-0P 303153-47-1P 303153-48-2P 358359-37-2P
464171-71-9P 834866-81-8P 863423-73-8P 863423-74-9P 863423-75-0P
863423-83-0P 863423-84-1P 863423-85-2P 863423-87-4P 863423-88-5P
863423-89-6P 863423-90-9P 1007851-31-1P 1007851-51-5P
1007851-54-8P 1007851-56-0P 1007851-58-2P 1007851-75-3P
1007851-83-3P 1007851-87-7P 1007852-39-2P 1007852-44-9P
1007852-49-4P 1007852-52-9P 1007852-56-3P 1007852-59-6P
1007852-62-1P 1007852-69-8P 1007852-82-5P 1007852-94-9P
1007853-25-9P 1007853-31-7P 1007853-42-0P 1007853-47-5P
1007853-53-3P 1007853-60-2P 1007854-35-4P 1007854-58-1P
1007854-87-6P 1007854-93-4P 1007854-97-8P 1007855-01-7P
1009072-94-9P 1009072-97-2P 1009072-99-4P 1009073-01-1P
1009073-06-6P 1009073-10-2P 1009073-13-5P 1009073-19-1P
1009073-22-6P 1009073-24-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regio- and stereoselective total synthesis of benanomicin-pradimicin antibiotics via diastereoselective ring-opening, semi-pinacol cyclization, and glycosylation)

IT 116249-65-1P 116299-57-1P 135819-17-9P 863423-76-1P 863423-77-2P
1007851-45-7P 1007851-60-6P 1007852-35-8P 1007853-03-3P
1007854-02-5P 1007854-06-9P 1007854-12-7P 1007854-16-1P
1007854-20-7P 1007854-23-0P 1007854-31-0P 1007854-77-4P
1009075-12-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereoselective total synthesis of benanomicin-pradimicin antibiotics via diastereoselective ring-opening, semi-pinacol cyclization, and glycosylation)

L4 ANSWER 2 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 147:117809 CASREACT <<LOGINID::20090621>>
TITLE: Isoxazole-directed pinacol rearrangement: stereocontrolled approach to angular stereogenic centers
AUTHOR(S): Suzuki, Keisuke; Takikawa, Hiroshi; Hachisu, Yoshifumi; Bode, Jeffrey W.
CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology, SORST-JST Agency, 2-12-1 O-okayama, Meguro-ku, Tokyo, 152-8551, Japan
SOURCE: Angewandte Chemie, International Edition (2007), 46(18), 3252-3254
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(13) OF 105 ...W ===> AM...



W (13) AM
YIELD 96%

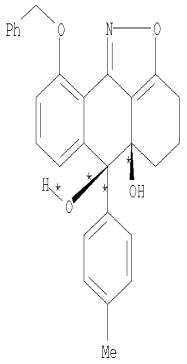
RX(13) RCT W 943151-36-8

STAGE(1)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C -> 0 deg C
SUBSTAGE(2) 3 hours, 0 deg C

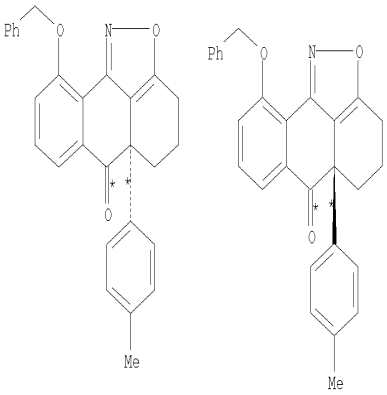
STAGE(2)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO AM 943151-37-9
NTE stereoselective

RX(14) OF 105 ...2 AC ===> AP + AQ



2 AC (14)



AP
YIELD 92%

AQ

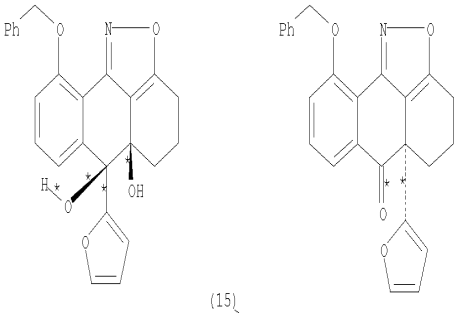
RX(14) RCT AC 943151-48-2

STAGE(1)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C -> 0 deg C
SUBSTAGE(2) 1 hour, 0 deg C

STAGE(2)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO AP 943151-53-9, AQ 943151-60-8
NTE stereoselective

RX(15) OF 105 ...AE ===> AR



AE (15)

AR
YIELD 90%

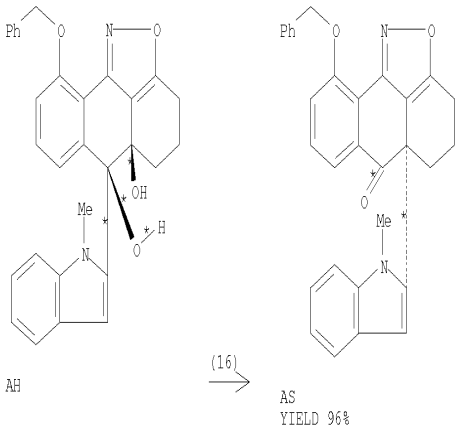
RX(15) RCT AE 943151-49-3

STAGE(1)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C -> 0 deg C
SUBSTAGE(2) 3 hours, 0 deg C

STAGE(2)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO AR 943151-54-0
NTE stereoselective

RX(16) OF 105 ...AH ===> AS



AH (16) AS
YIELD 96%

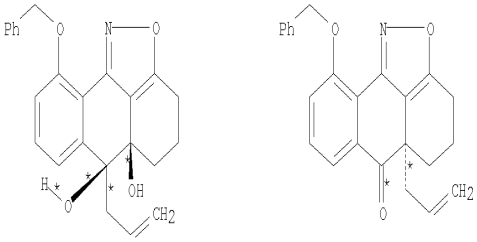
RX(16) RCT AH 943151-50-6

STAGE(1)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C -> 0 deg C
SUBSTAGE(2) 1.5 hours, 0 deg C

STAGE(2)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO AS 943151-55-1
NTE stereoselective

RX(17) OF 105 ...AJ ===> AT



AJ (17) AT
YIELD 95%

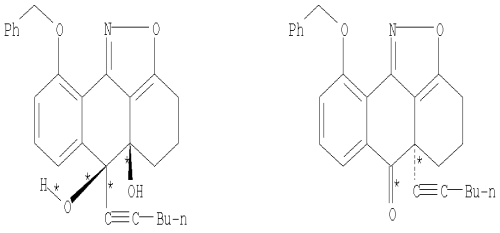
RX(17) RCT AJ 943151-51-7

STAGE(1)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C -> 0 deg C
SUBSTAGE(2) 2 hours, 0 deg C

STAGE(2)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO AT 943151-56-2
NTE stereoselective

RX(18) OF 105 ...AL ===> AU



AL (18) AU
YIELD 86%

RX(18) RCT AL 943151-52-8

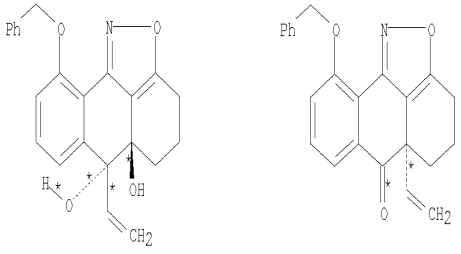
STAGE(1)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) -78 deg C -> 0 deg C
SUBSTAGE(2) 9 hours, 0 deg C

STAGE(2)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO AU 943151-57-3
NTE stereoselective

RX(21) OF 105 ...AA ===> AM...



AA (21) AM
YIELD 92%

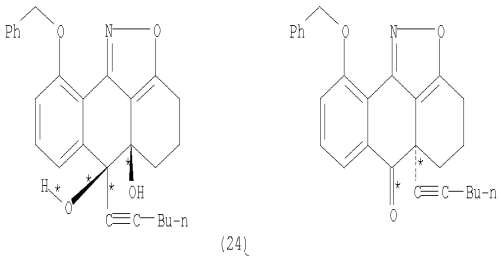
RX(21) RCT AA 943151-38-0

STAGE(1)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C -> 0 deg C
SUBSTAGE(2) 5 hours, 0 deg C

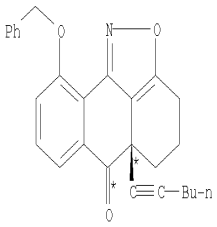
STAGE(2)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO AM 943151-37-9
NTE stereoselective

RX(24) OF 105 ...2 AL ===> AU + AZ



2 AL (24) AU
YIELD 82%



AZ

RX(24) RCT AL 943151-52-8

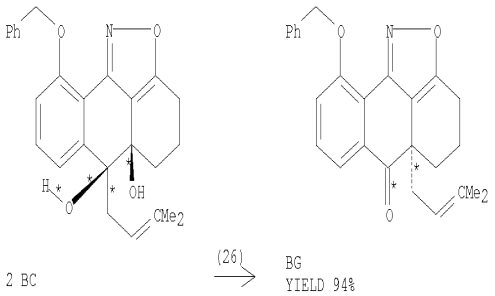
STAGE(1)
RGT BA 10210-68-1 Co2(CO)8
SOL 75-09-2 CH2Cl2
CON 2 hours, room temperature

STAGE(2)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> 0 deg C
SUBSTAGE(3) 5 hours, 0 deg C

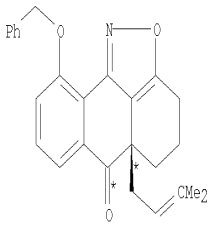
STAGE(3)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON 0 deg C

PRO AU 943151-57-3, AZ 943151-63-1
NTE stereoselective

RX(26) OF 105 ...2 BC ===> BG + BH



2 BC



BH

RX(26) RCT BC 943151-39-1

STAGE(1)
RGT AN 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> 0 deg C
SUBSTAGE(3) 0.5 hours, 0 deg C

STAGE(2)
RGT AO 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON 0 deg C

PRO BG 943151-40-4, BH 943151-59-5

TI Isoxazole-directed pinacol rearrangement: stereocontrolled approach to angular stereogenic centers

AB Underappreciated and neglected, isoxazoles are extremely good at stabilizing α cations. This ability is exploited in a method for the stereocontrolled introduction of angular substituents as found in polyketide-derived polycyclic natural products, such as 1. In a two-step process, the stereoselective addition of a nucleophile to the ketol 2 is followed by a regio- and stereospecific pinacol rearrangement. Bn = benzyl; R = allyl, aryl, heteroaryl, vinyl.

ST isoxazole pinacol rearrangement stereocontrol angular stereogenic center

IT Racemization
(acid; stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT Addition reaction
(nucleophilic; stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT Rearrangement
(pinacol; stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT Allylation
Asymmetric synthesis and induction
Molecular shape
Nucleophiles
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT Addition reaction
(stereoselective; stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT 943151-61-9P 943151-62-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(racemates; stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT 943151-47-1P 943151-59-5P 943151-60-8P 943151-63-1P
RL: BYP (Byproduct); PREP (Preparation)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT 10210-68-1
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); RGT (Reagent); PROC (Process); RACT (Reactant or reagent)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT 943151-35-7P 943151-36-8P 943151-38-0P 943151-39-1P 943151-42-6P 943151-44-8P 943151-45-9P 943151-46-0P 943151-48-2P 943151-49-3P 943151-50-6P 943151-51-7P 943151-52-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT 943151-37-9P 943151-40-4P 943151-53-9P 943151-54-0P 943151-55-1P 943151-56-2P 943151-57-3P 943151-58-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

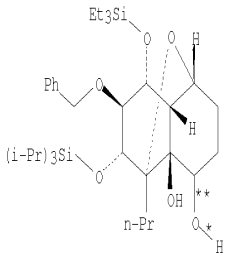
IT 92-52-4, Biphenyl, reactions 100-39-0, Benzyl bromide 109-72-8, n-Butyl lithium, reactions 110-00-9, Furan 503-60-6, 1-Chloro-3-methyl-2-butene 603-76-9, N-Methylindole 693-02-7, 1-Hexyne 1730-25-2, Allylmagnesium bromide 1826-67-1, Vinylmagnesium bromide 2417-95-0, 4-Methylphenyllithium 39637-74-6, (-)-Camphanic chloride 577975-53-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT 943151-41-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

IT 943151-43-7
RL: RGT (Reagent); RACT (Reactant or reagent)
(stereocontrolled approach to angular stereogenic centers on isoxazole-pinacol rearrangement)

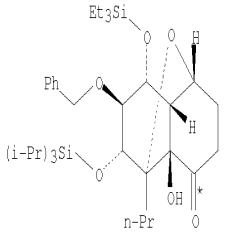
L4 ANSWER 3 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 144:51782 CASREACT <<LOGINID::20090621>>
TITLE: Synthesis of the A-B Subunit of Angelmicin B
AUTHOR(S): Lambert, William T.; Roush, William R.
CORPORATE SOURCE: Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109, USA
SOURCE: Organic Letters (2005), 7(24), 5501-5504
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(14) OF 300 ...BC ===> A...



BC

(14)



A

RX(14)

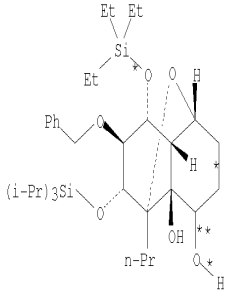
STAGE(1)
RGT AP 67-68-5 DMSO, AQ 79-37-8 (COCl)2
SOL 75-09-2 CH2Cl2
CON 10 minutes, -78 deg C

STAGE(2)
RCT BC 871268-88-1
SOL 75-09-2 CH2Cl2
CON 1 hour, -78 deg C

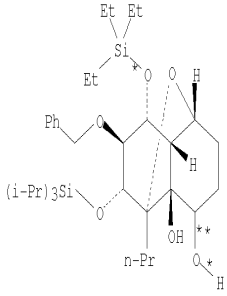
STAGE(3)
RGT P 121-44-8 Et3N
CON -78 deg C -> room temperature

PRO A 871268-89-2
NTE yield over two stages is 59%, Swern oxidation

RX(36) OF 300 COMPOSED OF RX(14), RX(1)
RX(36) 2 BC ===> B + C

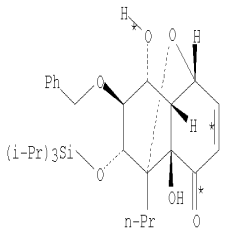


BC

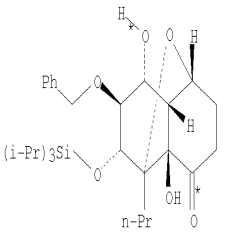


BC

2
STEPS



B
YIELD 61%(88)



C
YIELD 61%(12)

RX(14)

STAGE(1)

RGT AP 67-68-5 DMSO, AQ 79-37-8 (COCl)2
SOL 75-09-2 CH2Cl2
CON 10 minutes, -78 deg C

STAGE(2)
RGT BC 871268-88-1
SOL 75-09-2 CH2Cl2
CON 1 hour, -78 deg C

STAGE(3)
RGT P 121-44-8 Et3N
CON -78 deg C -> room temperature

PRO A 871268-89-2
NTE yield over two stages is 59%, Swern oxidation

RX(1) RCT A 871268-89-2

STAGE(1)
RGT D 5707-04-0 PhSeCl
CAT 7647-01-0 HCl
SOL 141-78-6 AcOEt
CON 6 hours, room temperature

STAGE(2)
RGT E 7732-18-5 Water
CON room temperature

STAGE(3)
RGT F 110-86-1 Pyridine, G 7722-84-1 H2O2
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

PRO B 871268-70-1, C 871268-90-5
NTE yield over 16 steps from the benzhydryldimethylsilyl substituted allene is 2%

ST asym synthesis AB subunit angelmicin formal three component coupling; THF prepn stereoselective annulation allylsilane aldehyde intramol aldol pinacol

IT Coupling reaction
(pinacol; synthesis of the A-B subunit of angelmicin B via)

L4 ANSWER 4 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 143:306299 CASREACT <<LOGINID::20090621>>
TITLE: Preparation of polycyclic ketones having anthraisoxazole structure by pinacol rearrangement of diols
INVENTOR(S): Suzuki, Keisuke
PATENT ASSIGNEE(S): Japan Science and Technology Agency, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005255592	A	20050922	JP 2004-67741	20040310
JP 4219289	B2	20090204		
WO 2005095422	A1	20051013	WO 2005-JP4723	20050310

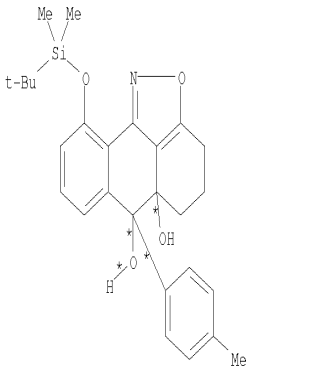
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1724274	A1	20061122	EP 2005-720958	20050310
R: DE, FR, GB				
US 20070149786	A1	20070628	US 2006-591974	20060908

PRIORITY APPLN. INFO.: JP 2004-67741 20040310
WO 2005-JP4723 20050310

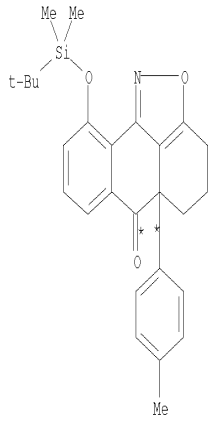
OTHER SOURCE(S): MARPAT 143:306299

RX(2) OF 3 ...C ===> I



(2)

C



I
YIELD 99%

RX(2) RCT C 864951-74-6

STAGE(1)
RGT J 109-63-7 BF3-Et2O
SOL 75-09-2 CH2Cl2
CON 30 minutes, 0 deg C

STAGE(2)
RGT K 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO I 864951-75-7

TI Preparation of polycyclic ketones having anthraisoxazole structure by pinacol rearrangement of diols

ST oxotetrahydroanthraisoxazole prepn; tollyldihydroxytetrahydroanthraisoxazole pinacol rearrangement Lewis acid catalyst

IT Sulfonic acids, uses
RL: CAT (Catalyst use); USES (Uses)
(alkanesulfonic; preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT Rearrangement
(pinacol; preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT Ketones, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(polycyclic; preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT Rearrangement catalysts
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT Acids, uses
Carboxylic acids, uses
Lewis acids
RL: CAT (Catalyst use); USES (Uses)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT 106-38-7, 4-Bromotoluene
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation of; preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT 109-63-7, Boron trifluoride-diethyl ether complex 7647-01-0, Hydrochloric acid, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT 864951-74-6P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT 864951-75-7P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT 60-29-7, Diethyl ether, uses 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-64-1, Dimethyl ketone, uses 67-66-3, Chloroform, uses 68-12-2, N,N-Dimethylformamide, uses 71-43-2, Benzene, uses 75-01-4, Chloroethylene, uses 75-05-8, Acetonitrile, uses 75-09-2, Dichloromethane, uses 108-88-3, Toluene, uses 109-99-9, Tetrahydrofuran, uses 110-71-4, 1,2-Dimethoxyethane 123-91-1, 1,4-Dioxane, uses 7732-18-5, Water, uses 25323-30-2, Dichloroethylene
RL: NUU (Other use, unclassified); USES (Uses)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT 864951-73-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

IT 2417-95-0P, p-Tolyllithium
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of polycyclic ketones having anthraisoxazole structure by catalytic pinacol-type rearrangement of diols)

L4 ANSWER 5 OF 11 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:336478 CASREACT <<LOGINID::20090621>>

TITLE: To seek an approach toward the chemical conversion of C19-diterpenoid alkaloids to taxoids

AUTHOR(S): Wang, Feng-Peng; Xu, Liang

CORPORATE SOURCE: Department of Chemistry of Medicinal Natural Products, West China College of Pharmacy, Sichuan University, Chengdu, 610041, Peop. Rep. China

SOURCE: Tetrahedron (2005), 61(8), 2149-2167
CODEN: TETRAB; ISSN: 0040-4020

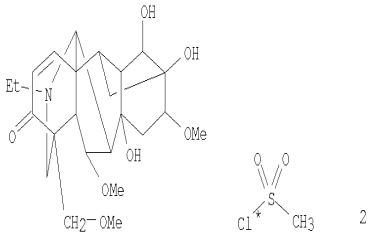
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

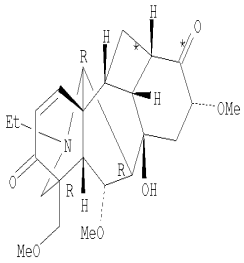
LANGUAGE: English

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(58) OF 154 COMPOSED OF RX(26), RX(27)
RX(58) BH + AU ===> BK



BH AU 2 STEPS

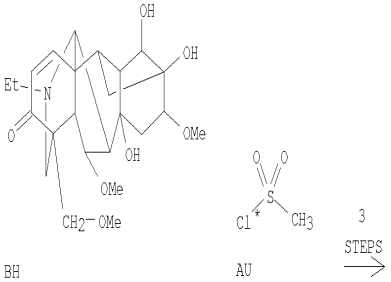


BK
YIELD 90%

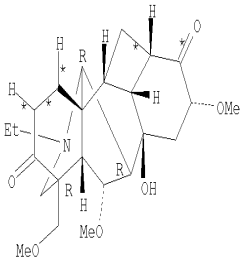
RX(26) RCT BH 286838-49-1, AU 124-63-0
PRO BJ 481687-46-1
SOL 110-86-1 Pyridine
CON 1.5 hours, room temperature
NTE regioselective

RX(27) RCT BJ 481687-46-1
RGT AT 1310-73-2 NaOH
PRO BK 481687-47-2
SOL 68-12-2 DMF
CON 30 minutes, reflux
NTE key step, semipinacol rearrangement

RX(93) OF 154 COMPOSED OF RX(26), RX(27), RX(28)
RX(93) BH + AU ===> BM



BH AU 3 STEPS



BM
YIELD 100%

RX(26) RCT BH 286838-49-1, AU 124-63-0
PRO BJ 481687-46-1
SOL 110-86-1 Pyridine
CON 1.5 hours, room temperature
NTE regioselective

RX(27) RCT BJ 481687-46-1
RGT AT 1310-73-2 NaOH
PRO BK 481687-47-2
SOL 68-12-2 DMF
CON 30 minutes, reflux
NTE key step, semipinacol rearrangement

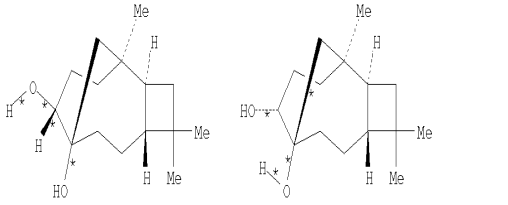
RX(28) RCT BK 481687-47-2
RGT BN 1333-74-0 H2
PRO BM 481687-50-7
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 1 hour, room temperature

AB This study, as a part of conversion of the C19-diterpenoid alkaloids to the taxoids, described the search of a suitable route to the key intermediate through four approaches. In these cases, a new and efficient approach (CAB) toward the synthesis of the vital intermediates I (R = H) or I (R = Ac) has been developed. The key steps in the synthesis include the use of a semi-pinacol rearrangement, carbon-nitrogen bond cleavage, and HIO4 oxidative bond cleavages.

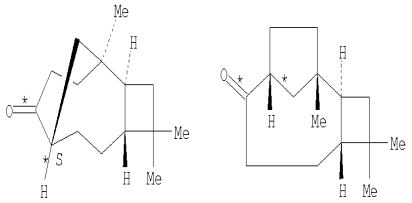
IT Rearrangement
(pinacol, semi-pinacol rearrangement; chemical conversion of C19-diterpenoid alkaloids to taxoids)

L4 ANSWER 6 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 142:176958 CASREACT <<LOGINID::20090621>>
TITLE: Synthesis of isocaryolane sesquiterpenes with potential antifungal activity with respect to Botrytis cinerea
AUTHOR(S): Racero, Juan Carlos; Collado, Isidro Gonzalez; Macias, Antonio Jose
CORPORATE SOURCE: Facultad de Ciencias Quimicas. Laboratorio de Sintesis Organica, Universidad Autonoma de San Luis Potosi, San Luis Potosi, 78210, Mex.
SOURCE: Revista de la Sociedad Quimica de Mexico (2004), 48(1), 58-66
CODEN: RSQMAN; ISSN: 0583-7693
PUBLISHER: Sociedad Quimica de Mexico
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 33 2 M ===> E + N...



M M



E N

RX(4) RCT M 99805-54-6

STAGE(1)
SOL 108-88-3 PhMe

STAGE(2)
RGT O 603-35-0 PPh3

STAGE(3)
CAT 1972-28-7 EtO2CN:NCO2Et
SOL 75-09-2 CH2Cl2

PRO E 203437-38-1, N 248918-62-9

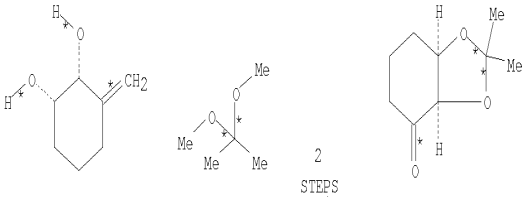
AB Sesquiterpenes with isocaryolane skeleton represent potential antifungal compds. because they possess a structural similarity to the phytotoxic metabolites produced by Botrytis cinerea. Isocaryolanes with functionality at C-8 and C-9 were prepared by rearrangement of caryophyllene derivs. and pinacol rearrangements of the resulting isocaryolane derivs. under Mitsunobu conditions. Isocaryolane alc. I showed interesting activity when tested in vitro against B. cinerea.

ST isocaryolane sesquiterpene synthesis pinacol rearrangement fungicidal activity

IT Rearrangement
(pinacol; synthesis of isocaryolane sesquiterpenes with potential antifungal activity with respect to Botrytis cinerea)

L4 ANSWER 7 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 141:156841 CASREACT <<LOGINID::20090621>>
TITLE: Intramolecular chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dicarbonyls
AUTHOR(S): Groth, Ulrich; Jung, Marc; Vogel, Till
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Konstanz, Konstanz, 78457, Germany
SOURCE: Synlett (2004), (6), 1054-1058
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(26) OF 50 COMPOSED OF RX(5), RX(6)
RX(26) B + T ===> X



B T X

RX(5) RCT B 728878-58-8, T 77-76-9
RGT V 24057-28-1 Pyridinium tosylate
PRO U 728878-66-8
SOL 67-64-1 Me2CO

CON room temperature

RX(6) RCT U 728878-66-8

STAGE(1)
RGT Y 10028-15-6 Ozone
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

STAGE(2)
RGT Z 75-18-3 Me2S

PRO X 146388-16-1

TI Intramolecular chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dicarbonyls

ST diastereoselective prepn cyclic diol; pinacol cross coupling methylene dicarbonyl chromium catalyst

IT Glycols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclic; diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT Stereoselective synthesis
(diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT Dialdehydes
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT Aldehydes, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(oxo; diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT Coupling reaction
(pinacol, diastereoselective; diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT Coupling reaction catalysts
(pinacol; diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT 10025-73-7, Chromium chloride (CrCl3)
RL: CAT (Catalyst use); USES (Uses)
(diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT 110-83-8, Cyclohexene, reactions 628-92-2, Cycloheptene 930-68-7, 2-Cyclohexenone 931-88-4, Cyclooctene
RL: RCT (Reactant); RACT (Reactant or reagent)
(diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT 55489-11-7P 60090-77-9P 146388-16-1P 148315-77-9P 728878-54-4P 728878-55-5P 728878-56-6P 728878-57-7P 728878-58-8P 728878-66-8P 728878-67-9P 728878-68-0P 728878-69-1P 728878-72-6P 728878-73-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT 728878-59-9P 728878-60-2P 728878-61-3P 728878-62-4P 728878-63-5P 728878-64-6P 728878-65-7P 728878-70-4P 728878-71-5P 728878-74-8P 728878-75-9P 728878-76-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT 7439-96-5, Manganese, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(reducing agent; diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

IT 75-77-4, Trimethylsilyl chloride, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(scavenger; diastereoselective preparation of cyclic diols by chromium(II)-catalyzed pinacol cross coupling of 2-methylene-α,ω-dialdehydes and -ketones)

L4 ANSWER 8 OF 11 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:245742 CASREACT <<LOGINID::20090621>>

TITLE: Synthesis, structure, and properties of a dibenzo-ortho-terphenoquinone. The first o-terphenoquinone derivative

AUTHOR(S): Kurata, Hiroyuki; Takehara, Yuko; Kawase, Takeshi; Oda, Masaji

CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Osaka University, Osaka, 560-0043, Japan

SOURCE: Chemistry Letters (2003), 32(6), 538-539
CODEN: CMLTAG; ISSN: 0366-7022

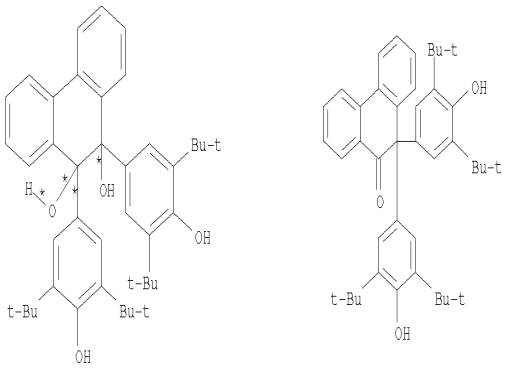
PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 15 ...C ===> F...

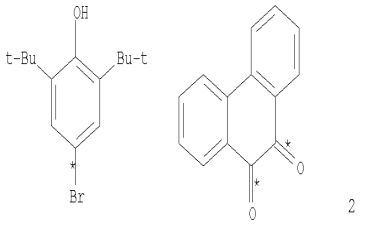


C (2) → F

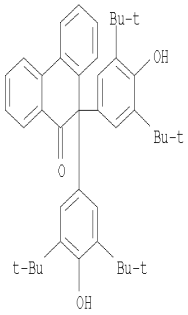
YIELD 75%

RX(2) RCT C 596796-45-1
       PRO F 596796-46-2
       CAT 76-05-1 F3CCO2H
       SOL 64-19-7 AcOH
       CON 1 hour, room temperature
       NTE pinacol rearrangement

RX(6) OF 15 COMPOSED OF RX(1), RX(2)
RX(6) 2 A + B ===> F



2 A B 2 STEPS



F
YIELD 75%

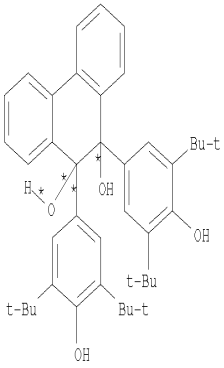
RX(1) RCT A 1139-52-2

STAGE(1)
RGT D 594-19-4 t-BuLi
SOL 60-29-7 Et20
CON 1 hour, 0 deg C

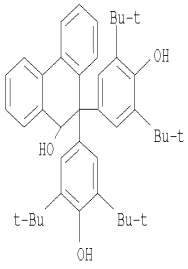
STAGE(2)
RCT B 84-11-7
SOL 60-29-7 Et20
PRO C 596796-45-1
NTE THF as solvent did not yield product at all

RX(2) RCT C 596796-45-1
       PRO F 596796-46-2
       CAT 76-05-1 F3CCO2H
       SOL 64-19-7 AcOH
       CON 1 hour, room temperature
       NTE pinacol rearrangement

RX(7) OF 15 COMPOSED OF RX(2), RX(3)
RX(7) C ===> I



C 2 STEPS

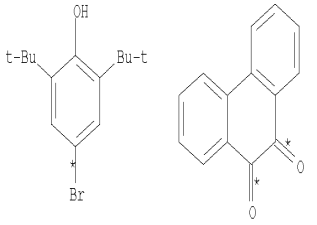


I
YIELD 81%

RX(2) RCT C 596796-45-1
       PRO F 596796-46-2
       CAT 76-05-1 F3CCO2H
       SOL 64-19-7 AcOH
       CON 1 hour, room temperature
       NTE pinacol rearrangement

RX(3) RCT F 596796-46-2
       RGT J 16853-85-3 LiAlH4
       PRO I 670218-75-4
       SOL 109-99-9 THF
       CON 1.5 hours, reflux

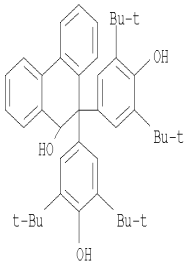
RX(10) OF 15 COMPOSED OF RX(1), RX(2), RX(3)
RX(10) 2 A + B ===> I



2 A

B

3
STEPS



I
YIELD 81%

RX(1) RCT A 1139-52-2

STAGE(1)
RGT D 594-19-4 t-BuLi
SOL 60-29-7 Et2O
CON 1 hour, 0 deg C

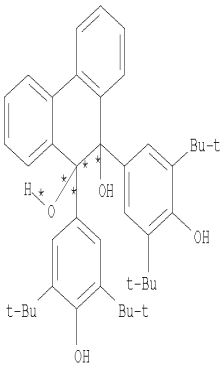
STAGE(2)
RCT B 84-11-7
SOL 60-29-7 Et2O

PRO C 596796-45-1
NTE THF as solvent did not yield product at all

RX(2) RCT C 596796-45-1
PRO F 596796-46-2
CAT 76-05-1 F3CCO2H
SOL 64-19-7 AcOH
CON 1 hour, room temperature
NTE pinacol rearrangement

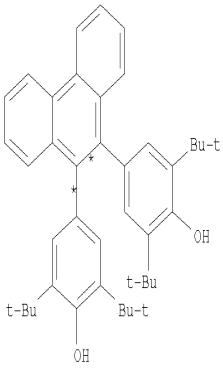
RX(3) RCT F 596796-46-2
RGT J 16853-85-3 LiAlH4
PRO I 670218-75-4
SOL 109-99-9 THF
CON 1.5 hours, reflux

RX(11) OF 15 COMPOSED OF RX(2), RX(3), RX(5)
RX(11) C ===> L



C

3
STEPS



L
YIELD 74%

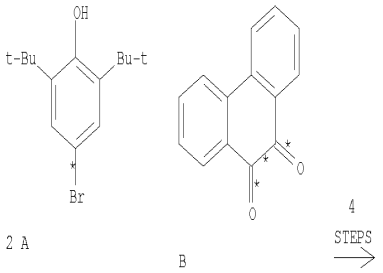
RX(2) RCT C 596796-45-1
PRO F 596796-46-2
CAT 76-05-1 F3CCO2H
SOL 64-19-7 AcOH
CON 1 hour, room temperature
NTE pinacol rearrangement

RX(3) RCT F 596796-46-2
RGT J 16853-85-3 LiAlH4

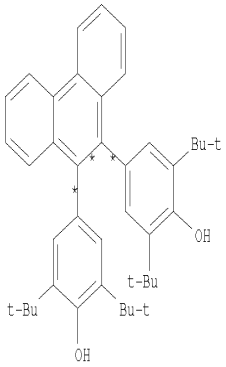
PRO I 670218-75-4
SOL 109-99-9 THF
CON 1.5 hours, reflux

RX(5) RCT I 670218-75-4
PRO L 596796-47-3
CAT 7553-56-2 I2
SOL 64-19-7 AcOH
CON 1.5 hours, reflux

RX(12) OF 15 COMPOSED OF RX(1), RX(2), RX(3), RX(5)
RX(12) 2 A + B ===> L



2 A B



L
YIELD 74%

RX(1) RCT A 1139-52-2

STAGE(1)
RGT D 594-19-4 t-BuLi
SOL 60-29-7 Et2O
CON 1 hour, 0 deg C

STAGE(2)
RCT B 84-11-7
SOL 60-29-7 Et2O

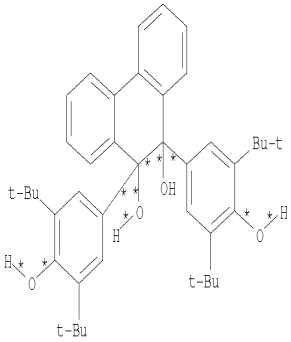
PRO C 596796-45-1
NTE THF as solvent did not yield product at all

RX(2) RCT C 596796-45-1
PRO F 596796-46-2
CAT 76-05-1 F3CCO2H
SOL 64-19-7 AcOH
CON 1 hour, room temperature
NTE pinacol rearrangement

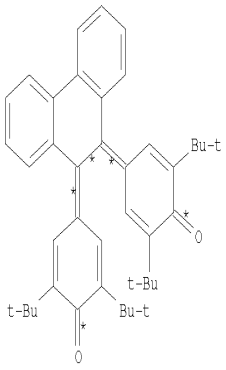
RX(3) RCT F 596796-46-2
RGT J 16853-85-3 LiAlH4
PRO I 670218-75-4
SOL 109-99-9 THF
CON 1.5 hours, reflux

RX(5) RCT I 670218-75-4
PRO L 596796-47-3
CAT 7553-56-2 I2
SOL 64-19-7 AcOH
CON 1.5 hours, reflux

RX(14) OF 15 COMPOSED OF RX(2), RX(3), RX(5), RX(4)
RX(14) C ===> M



C



M
YIELD 99%

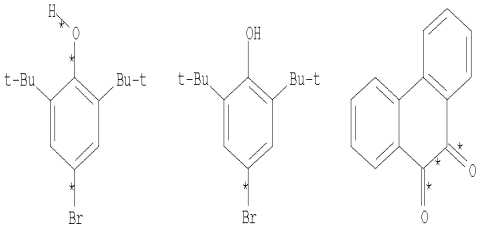
RX(2) RCT C 596796-45-1
PRO F 596796-46-2
CAT 76-05-1 F3CCO2H
SOL 64-19-7 AcOH
CON 1 hour, room temperature
NTE pinacol rearrangement

RX(3) RCT F 596796-46-2
RGT J 16853-85-3 LiAlH4
PRO I 670218-75-4
SOL 109-99-9 THF
CON 1.5 hours, reflux

RX(5) RCT I 670218-75-4
PRO L 596796-47-3
CAT 7553-56-2 I2
SOL 64-19-7 AcOH
CON 1.5 hours, reflux

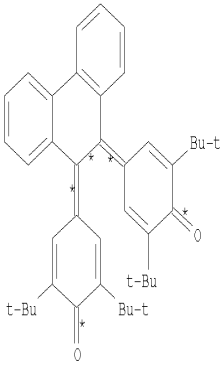
RX(4) RCT L 596796-47-3
RGT N 13746-66-2 K3Fe(CN)6, O 1310-58-3 KOH
PRO M 596796-44-0
SOL 7732-18-5 Water, 71-43-2 Benzene
CON 3 days, room temperature

RX(15) OF 15 COMPOSED OF RX(1), RX(2), RX(3), RX(5), RX(4)
RX(15) 2 A + B ===> M



A A B

5
STEPS



M
YIELD 99%

RX(1) RCT A 1139-52-2

STAGE(1)
RGT D 594-19-4 t-BuLi
SOL 60-29-7 Et2O
CON 1 hour, 0 deg C

STAGE(2)
RCT B 84-11-7
SOL 60-29-7 Et2O

PRO C 596796-45-1
NTE THF as solvent did not yield product at all

RX(2) RCT C 596796-45-1

PRO F 596796-46-2
CAT 76-05-1 F3CCO2H
SOL 64-19-7 AcOH
CON 1 hour, room temperature
NTE pinacol rearrangement

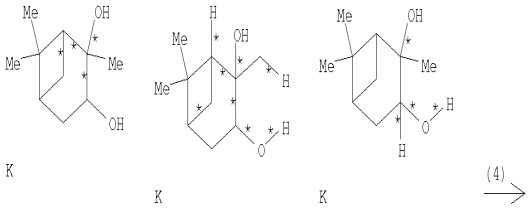
RX(3) RCT F 596796-46-2
RGT J 16853-85-3 LiAlH4
PRO I 670218-75-4
SOL 109-99-9 THF
CON 1.5 hours, reflux

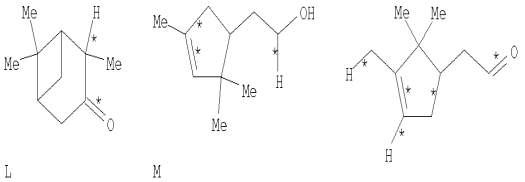
RX(5) RCT I 670218-75-4
PRO L 596796-47-3
CAT 7553-56-2 I2
SOL 64-19-7 AcOH
CON 1.5 hours, reflux

RX(4) RCT L 596796-47-3
RGT N 13746-66-2 K3Fe(CN)6, O 1310-58-3 KOH
PRO M 596796-44-0
SOL 7732-18-5 Water, 71-43-2 Benzene
CON 3 days, room temperature

L4 ANSWER 9 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 137:108883 CASREACT <<LOGINID::20090621>>
TITLE: Fe-substituted molecular sieves as catalysts in the liquid phase pinacol rearrangement
AUTHOR(S): Hsien, Michelle; Sheu, Horng-Tay; Lee, Tao; Cheng, Soofin; Lee, Jyh-Fu
CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan
SOURCE: Journal of Molecular Catalysis A: Chemical (2002), 181(1-2), 189-200
CODEN: JMCCF2; ISSN: 1381-1169
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 4 3 K ===> L + M + N





L
YIELD 54%

M
YIELD 35%

N
YIELD 11%

RX(4) RCT K 53404-49-2
PRO L 18358-53-7, M 4605-50-9, N 91819-58-8
SOL 108-88-3 PhMe
NTE FeMCM-41 used as cat.,alternative cat. shown

TI Fe-substituted molecular sieves as catalysts in the liquid phase pinacol rearrangement

AB Pinacol-type rearrangement reactions in toluene were catalyzed by iron-substituted mol. sieves of different porous structures, including AlPO4-5, ZSM-5 of micropores and MCM-41 of mesopores. Iron(III)-substituted in the framework of the mol. sieves was found to be the active center for the pinacol rearrangement. The catalytic activity was found to have no correlation with the acidity. Ten vicinal diol reactants with various alkyl or aryl substitution were examined The results showed that AlPO4-5 mol. sieve containing 0.5-2% Fe was the most active in catalyzing the pinacol rearrangement of 2,3-dimethyl-2,3-butanediol. On the other hand, Fe-substituted MCM-41 with relatively large pores was most active in catalyzing the rearrangement of large mols. such as 2,3-pinanediol and 2,3-diphenyl-1,2-ethanediol. All these mol. sieves were not catalytically active in the rearrangement of the vicinal diol compds. of high polarity. This was attributed to the fact that polar mols. would cover the catalyst surfaces and deactivate the catalysts. The migrating preference of the substitution groups was dependent on the catalysts and was different from that observed on acid-catalyzed reactions.

ST pinacol rearrangement iron mol sieve

IT Aluminophosphate zeolites
RL: CAT (Catalyst use); USES (Uses)
(APO 5, APO-5; iron-substituted mol. sieves as catalysts in liquid phase pinacol rearrangement)

IT Molecular sieves
(iron-substituted mol. sieves as catalysts in liquid phase pinacol rearrangement)

IT Zeolite MCM-41
Zeolite ZSM-5
RL: CAT (Catalyst use); USES (Uses)
(iron-substituted mol. sieves as catalysts in liquid phase pinacol rearrangement)

IT Rearrangement catalysts
(pinacol; iron-substituted mol. sieves as catalysts in liquid phase pinacol rearrangement)

IT 7439-89-6, Iron, uses 7784-30-7
RL: CAT (Catalyst use); USES (Uses)
(iron-substituted mol. sieves as catalysts in liquid phase pinacol rearrangement)

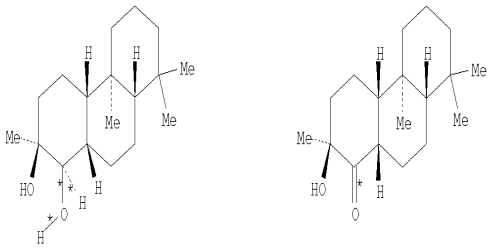
IT 76-09-5, Pinacol 93-56-1, 1-Phenyl-1,2-ethanediol 492-70-6, 1,2-Diphenyl-1,2-ethanediol 53404-49-2, 2,3-Pinanediol
RL: RCT (Reactant); RACT (Reactant or reagent)

(iron-substituted mol. sieves as catalysts in liquid phase pinacol rearrangement)

IT 75-97-8P, Pinacolone 122-78-1P, Phenylacetaldehyde 451-40-1P, Benzyl phenyl ketone 947-91-1P, Diphenylacetaldehyde 4605-50-9P 18358-53-7P 91819-58-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(iron-substituted mol. sieves as catalysts in liquid phase pinacol rearrangement)

L4 ANSWER 10 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 137:33426 CASREACT <<LOGINID::20090621>>
TITLE: Cyclization of bicyclic diterpenes promoted by SmI2. synthesis of tri- and tetracyclic diterpenes
AUTHOR(S): Marcos, Isidro S.; Moro, Rosalina F.; Carballares M., Santiago; Urones, Julio G.
CORPORATE SOURCE: Dept. de Quimica Organica, Universidad de Salamanca, Salamanca, 37008, Spain
SOURCE: Synlett (2002), (3), 458-462
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

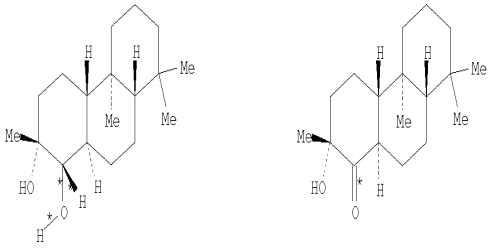
RX(11) OF 114 ...U ===> AL



U (11) AL
YIELD 88%

RX(11) RCT U 437654-90-5
RGT S 67-68-5 DMSO, R 79-37-8 (COCl)2, T 121-44-8 Et3N
PRO AL 437655-03-3
SOL 75-09-2 CH2Cl2
NTE Swern oxidn.

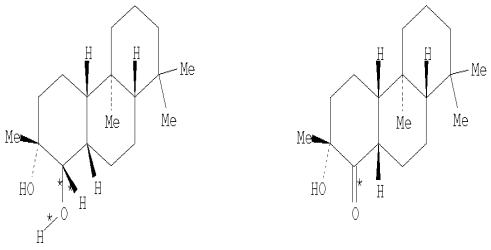
RX(12) OF 114 ...AI ===> AM



AI (12) AM
YIELD 79%

RX(12) RCT AI 437654-96-1
RGT S 67-68-5 DMSO, R 79-37-8 (COCl)2, T 121-44-8 Et3N
PRO AM 437655-05-5
SOL 75-09-2 CH2Cl2

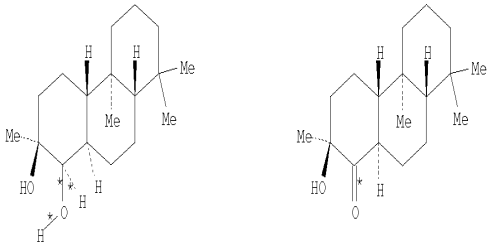
RX(13) OF 114 ...V ===> AN



V (13) AN
YIELD 84%

RX(13) RCT V 437654-92-7
RGT S 67-68-5 DMSO, R 79-37-8 (COCl)2, T 121-44-8 Et3N
PRO AN 437655-07-7
SOL 75-09-2 CH2Cl2

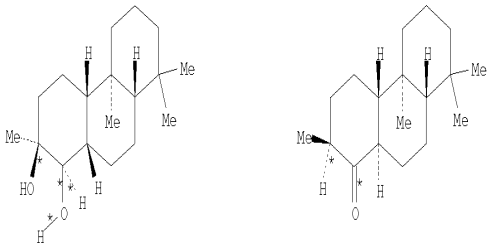
RX(14) OF 114 ...AK ===> AO



AK (14) → AO, YIELD 88%

RX(14) RCT AK 437654-99-4
RGT S 67-68-5 DMSO, R 79-37-8 (COCl)2, T 121-44-8 Et3N
PRO AO 437655-09-9
SOL 75-09-2 CH2Cl2

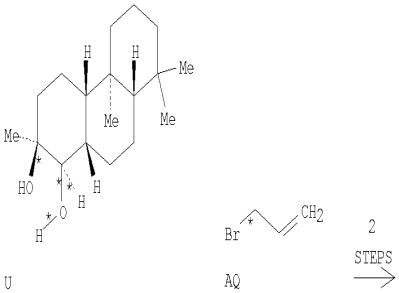
RX(15) OF 114 ...U ===> AP...



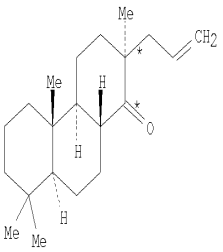
U (15) → AP, YIELD 90%

RX(15) RCT U 437654-90-5
RGT AB 104-15-4 TsOH
PRO AP 437655-11-3
SOL 109-99-9 THF

RX(36) OF 114 COMPOSED OF RX(15), RX(16)
RX(36) U + AQ ===> AR



U + AQ (2 STEPS) →

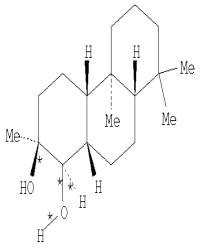


AR
YIELD 80%

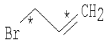
RX(15) RCT U 437654-90-5
RGT AB 104-15-4 TsOH
PRO AP 437655-11-3
SOL 109-99-9 THF

RX(16) RCT AP 437655-11-3, AQ 106-95-6
RGT AS 40949-94-8 K [N(SiMe3)2]
PRO AR 437655-13-5
SOL 109-99-9 THF

RX(78) OF 114 COMPOSED OF RX(15), RX(16), RX(17)
RX(78) U + AQ ===> AT

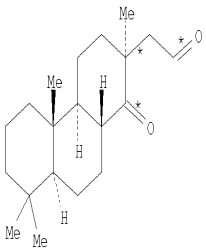


U



AQ

3
STEPS



AT
YIELD 90%

RX(15) RCT U 437654-90-5
RGT AB 104-15-4 TsOH
PRO AP 437655-11-3
SOL 109-99-9 THF

RX(16) RCT AP 437655-11-3, AQ 106-95-6
RGT AS 40949-94-8 K [N(SiMe3)2]
PRO AR 437655-13-5
SOL 109-99-9 THF

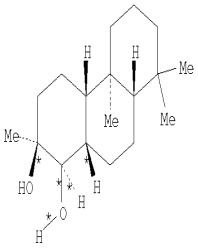
RX(17) RCT AR 437655-13-5

STAGE(1)
RGT C 20816-12-0 OsO4, D 7529-22-8 Me-morpholineoxide
SOL 75-65-0 t-BuOH, 109-99-9 THF, 7732-18-5 Water

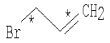
STAGE(2)
RGT AU 7790-28-5 NaIO4
SOL 109-99-9 THF, 7732-18-5 Water

PRO AT 437655-15-7

RX(81) OF 114 COMPOSED OF RX(15), RX(16), RX(17), RX(18)
RX(81) U + AQ ===> AV

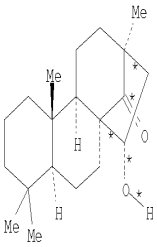


U



AQ

4
STEPS



AV
YIELD 75%

RX(15) RCT U 437654-90-5
RGT AB 104-15-4 TsOH
PRO AP 437655-11-3
SOL 109-99-9 THF

RX(16) RCT AP 437655-11-3, AQ 106-95-6
RGT AS 40949-94-8 K [N(SiMe3)2]
PRO AR 437655-13-5
SOL 109-99-9 THF

RX(17) RCT AR 437655-13-5

STAGE(1)
RGT C 20816-12-0 OsO4, D 7529-22-8 Me-morpholineoxide
SOL 75-65-0 t-BuOH, 109-99-9 THF, 7732-18-5 Water

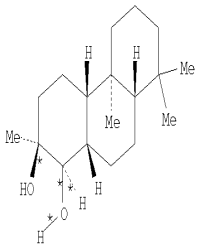
STAGE(2)
RGT AU 7790-28-5 NaIO4
SOL 109-99-9 THF, 7732-18-5 Water

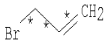
PRO AT 437655-15-7

RX(18) RCT AT 437655-15-7
RGT AW 1310-58-3 KOH

PRO AV 68270-44-0
SOL 67-56-1 MeOH
NTE stereoselective

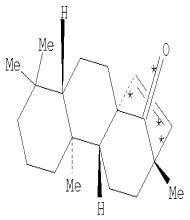
RX(110) OF 114 COMPOSED OF RX(15), RX(16), RX(17), RX(18), RX(19)
RX(110) U + AQ ===> AX





5 STEPS

U AQ



AX
YIELD 65%

RX(15) RCT U 437654-90-5
RGT AB 104-15-4 TsOH
PRO AP 437655-11-3
SOL 109-99-9 THF

RX(16) RCT AP 437655-11-3, AQ 106-95-6
RGT AS 40949-94-8 K [N(SiMe3)2]
PRO AR 437655-13-5
SOL 109-99-9 THF

RX(17) RCT AR 437655-13-5

STAGE(1)
RGT C 20816-12-0 OsO4, D 7529-22-8 Me-morpholineoxide
SOL 75-65-0 t-BuOH, 109-99-9 THF, 7732-18-5 Water

STAGE(2)
RGT AU 7790-28-5 NaIO4
SOL 109-99-9 THF, 7732-18-5 Water

PRO AT 437655-15-7

RX(18) RCT AT 437655-15-7
RGT AW 1310-58-3 KOH
PRO AV 68270-44-0
SOL 67-56-1 MeOH
NTE stereoselective

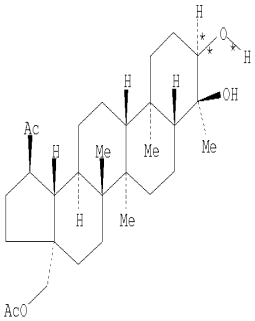
RX(19) RCT AV 68270-44-0
RGT AY 98-59-9 TsCl
PRO AX 52567-68-7
SOL 110-86-1 Pyridine

AB 15-Hibaen-14-one, a tetracyclic diterpene, was synthesized from zamoranic acid as starting material in an excellent yield and with total control of the stereochem. The key step was a SmI2 promoted pinacol cyclization.

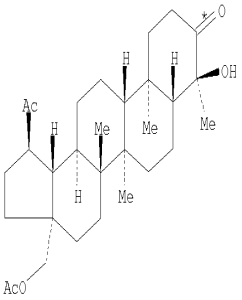
ST hibaenone synthesis zamoranic acid; pinacol cyclization samarium diiodide

L4 ANSWER 11 OF 11 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 137:6289 CASREACT <<LOGINID::20090621>>
TITLE: Preparation of a 24-Nor-1,4-dien-3-one Triterpene Derivative from Betulin: A New Route to 24-Nortriterpene Analogues
AUTHOR(S): Deng, Yonghong; Snyder, John K.
CORPORATE SOURCE: Department of Chemistry, Boston University, Boston, MA, 02215, USA
SOURCE: Journal of Organic Chemistry (2002), 67(9), 2864-2873 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 132 THERE ARE 132 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(9) OF 166 ...X ===> AA...



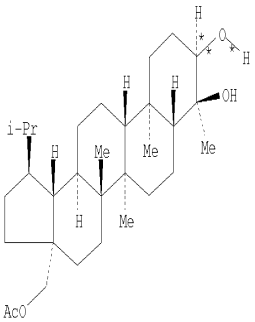
X (9)



AA
YIELD 73%

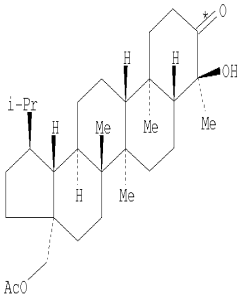
RX(9) RCT X 433336-17-5
PRO AA 433336-18-6
NTE stereoselective, swern oxidn.

RX(20) OF 166 ...AV ===> AW...



AV

(20)



AW
YIELD 79%

RX(20) RCT AV 433336-28-8
PRO AW 433336-30-2
NTE stereoselective, swern oxidn.

AB A new route to 24-nortriterpene derivs. with 2-hydroxy-Δ1,4-cyclohexadien-3-one A-rings, e.g. I, from triterpene precursors has been demonstrated beginning with betulin to prepare derivs. of betulinic acid. The key steps in the transformation are a Suarez cleavage of the A-ring with a subsequent SmI2-mediated pinacol -type coupling to reclose the A-ring following removal of the C-24 carbon by oxidative cleavage. Target compound I and a model were submitted to NCI for anticancer screening.

ST nortriterpene betulinic acid deriv asym synthesis oxidative cleavage reaction; Suarez bond cleavage nortriterpene betulinic acid deriv asym synthesis; pinacol type coupling nortriterpene betulinic acid deriv asym synthesis; anticancer agent nortriterpene betulinic acid deriv

IT Coupling reaction
(pinacol-type; preparation of a 24-nor-1,4-dien-3-one triterpene derivative via)

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	206.40	207.10
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.46	-5.46

FILE 'CASREACT' ENTERED AT 11:52:31 ON 21 JUN 2009

FILE CONTENT:1840 - 14 Jun 2009 VOL 150 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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************************************************************
*                                                          *
*     CASREACT now has more than 16.5 million reactions    *
*                                                          *
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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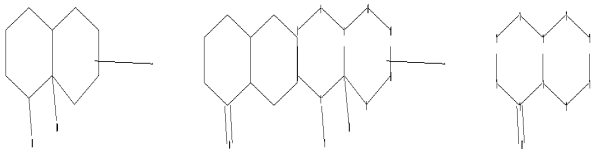
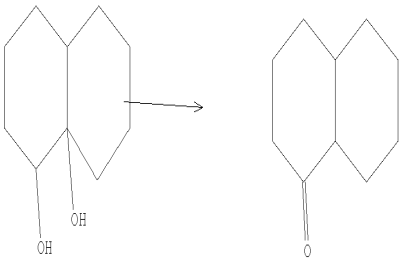


chain nodes :
7 17 21
ring nodes :
1 2 3 4 5 6 8 11 12 13 14 15 16 18 19 20 22 23 24 25
chain bonds :
1-7 6-21 11-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-18 6-8 8-20 11-12 11-16 12-13 13-14 14-15
15-16 15-22 16-25 18-19 19-20 22-23 23-24 24-25
exact/norm bonds :
1-2 1-6 1-7 2-3 4-5 5-6 5-18 6-8 6-21 8-20 11-16 11-17 12-13 13-14
14-15 15-16 15-22 16-25 18-19 19-20 22-23 23-24 24-25
exact bonds :
3-4 11-12

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom 19:Atom 20:Atom 21:CLASS
22:Atom 23:Atom
24:Atom 25:Atom
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l5 sss full
FULL SEARCH INITIATED 11:52:59 FILE 'CASREACT'
SCREENING COMPLETE - 119389 REACTIONS TO VERIFY FROM 6513 DOCUMENTS

100.0% DONE 119389 VERIFIED 163 HIT RXNS 49 DOCS
SEARCH TIME: 00.00.07

L6 49 SEA SSS FUL L5 (163 REACTIONS)

=> s l6 and pinacol
1580 PINACOL
154 PINACOLS
1613 PINACOL
(PINACOL OR PINACOLS)
L7 3 L6 AND PINACOL

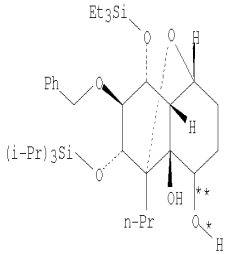
=> s l7 not l5
L7 MAY NOT BE USED HERE
The L-number entered was not created by a STRUCTURE or SCREEN command.

=> s l6 not l5
L6 MAY NOT BE USED HERE
The L-number entered was not created by a STRUCTURE or SCREEN command.

=> d l7 1-3 ibib hit

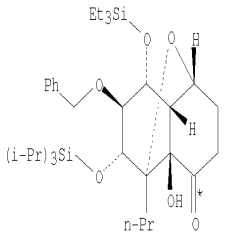
L7 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 144:51782 CASREACT <<LOGINID::20090621>>
TITLE: Synthesis of the A-B Subunit of Angelmicin B
AUTHOR(S): Lambert, William T.; Roush, William R.
CORPORATE SOURCE: Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109, USA
SOURCE: Organic Letters (2005), 7(24), 5501-5504
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS

RX(14) OF 300 ...BC ===> A...



BC

(14)



A

RX(14)

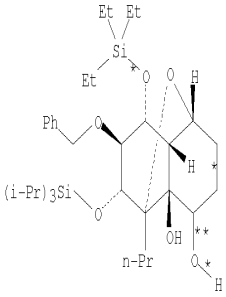
STAGE(1)
RGT AP 67-68-5 DMSO, AQ 79-37-8 (COCl)2
SOL 75-09-2 CH2Cl2
CON 10 minutes, -78 deg C

STAGE(2)
RCT BC 871268-88-1
SOL 75-09-2 CH2Cl2
CON 1 hour, -78 deg C

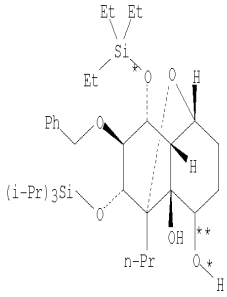
STAGE(3)
RGT P 121-44-8 Et3N
CON -78 deg C -> room temperature

PRO A 871268-89-2
NTE yield over two stages is 59%, Swern oxidation

RX(36) OF 300 COMPOSED OF RX(14), RX(1)
RX(36) 2 BC ===> B + C

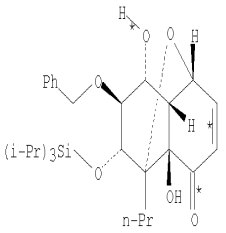


BC

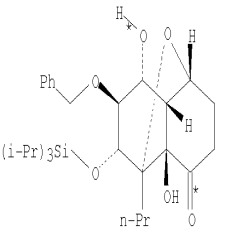


BC

2
STEPS



B
YIELD 61%(88)



C
YIELD 61%(12)

RX(14)

STAGE(1)
RGT AP 67-68-5 DMSO, AQ 79-37-8 (COCl)2
SOL 75-09-2 CH2Cl2
CON 10 minutes, -78 deg C

STAGE(2)
RCT BC 871268-88-1
SOL 75-09-2 CH2Cl2
CON 1 hour, -78 deg C

STAGE(3)
RGT P 121-44-8 Et3N
CON -78 deg C -> room temperature

PRO A 871268-89-2

NTE yield over two stages is 59%, Swern oxidation

RX(1) RCT A 871268-89-2

STAGE(1)
RGT D 5707-04-0 PhSeCl
CAT 7647-01-0 HCl
SOL 141-78-6 AcOEt
CON 6 hours, room temperature

STAGE(2)
RGT E 7732-18-5 Water
CON room temperature

STAGE(3)
RGT F 110-86-1 Pyridine, G 7722-84-1 H2O2
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

PRO B 871268-70-1, C 871268-90-5
NTE yield over 16 steps from the benzhydryldimethylsilyl substituted allene is 2%

ST asym synthesis AB subunit angelmicin formal three component coupling; THF prepn stereoselective annulation allylsilane aldehyde intramol aldol pinacol

IT Coupling reaction
(pinacol; synthesis of the A-B subunit of angelmicin B via)

L7 ANSWER 2 OF 3 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:71786 CASREACT <<LOGINID::20090621>>

TITLE: Synthetic study of aquayamycin. Part 3: first total synthesis

AUTHOR(S): Matsumoto, Takashi; Yamaguchi, Hiroki; Tanabe, Mitsujiro; Yasui, Yoshizumi; Suzuki, Keisuke

CORPORATE SOURCE: Department of Chemistry, Tokyo Institute of Technology, Japan Science and Technology Corporation (JST), Tokyo, 152-8551, Japan

SOURCE: Tetrahedron Letters (2000), 41(43), 8393-8396
CODEN: TELEAY; ISSN: 0040-4039

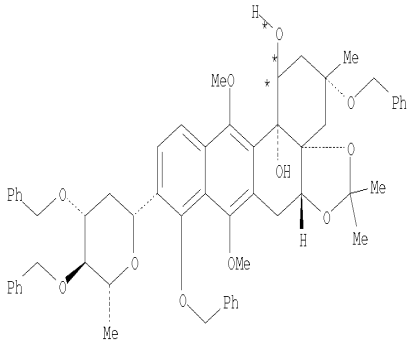
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

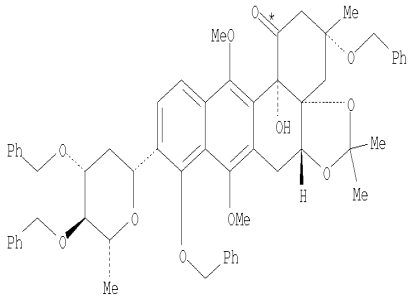
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 36 ...M ===> R...



M

(4)



R

YIELD 90%

RX(4) RCT M 314270-76-3

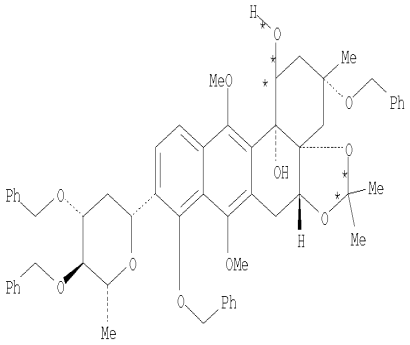
STAGE(1)
RGT S 79-37-8 (COCl)2, T 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT U 121-44-8 Et3N

PRO R 314270-77-4
NTE STEREOSELECTIVE

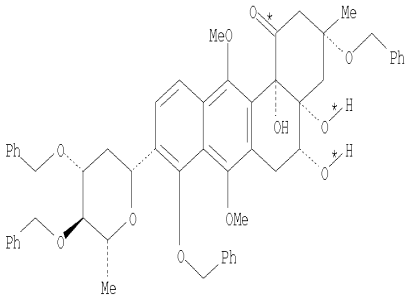
RX(12) OF 36 COMPOSED OF RX(4), RX(5)

RX(12) M ===> V



M

2
STEPS



V
YIELD 96%

RX(4) RCT M 314270-76-3

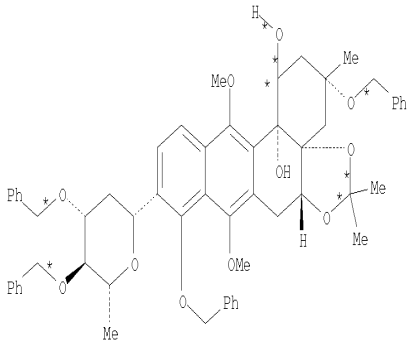
STAGE(1)
RGT S 79-37-8 (COCl)2, T 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT U 121-44-8 Et3N

PRO R 314270-77-4
NTE STEREOSELECTIVE

RX(5) RCT R 314270-77-4
RGT W 7664-93-9 H2SO4
PRO V 314270-83-2
SOL 7732-18-5 Water, 123-91-1 Dioxane
NTE STEREOSELECTIVE

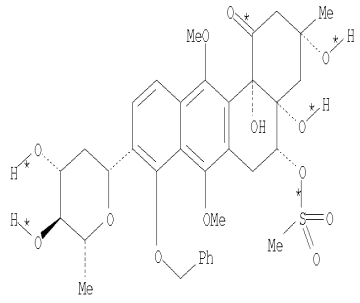
RX(21) OF 36 COMPOSED OF RX(4), RX(5), RX(8)
RX(21) M + AG ===> Z



M

AG

3
STEPS



Z
YIELD 79%

RX(4) RCT M 314270-76-3

STAGE(1)
RGT S 79-37-8 (COCl)2, T 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT U 121-44-8 Et3N

PRO R 314270-77-4
NTE STEREOSELECTIVE

RX(5) RCT R 314270-77-4
RGT W 7664-93-9 H2SO4
PRO V 314270-83-2
SOL 7732-18-5 Water, 123-91-1 Dioxane

NTE STEREOSELECTIVE

RX(8) RCT V 314270-83-2, AG 124-63-0

STAGE(1)
RGT AH 1122-58-3 4-DMAP, K 110-86-1 Pyridine
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT AC 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 141-78-6 AcOEt, 67-56-1 MeOH

STAGE(3)
RGT AI 100-39-0 PhCH2Br, AJ 534-17-8 Cs2CO3
SOL 68-12-2 DMF

PRO Z 314270-79-6
NTE STEREOSELECTIVE

AB The first total synthesis of aquayamycin has been accomplished. The crucial steps include (1) the Hauser reaction between 3-(phenylsulfonyl)phthalide and a cyclohexenone to make up the linear BCD tricycle, and (2) the intramol. pinacol coupling of a keto aldehyde to the full tetracyclic framework.

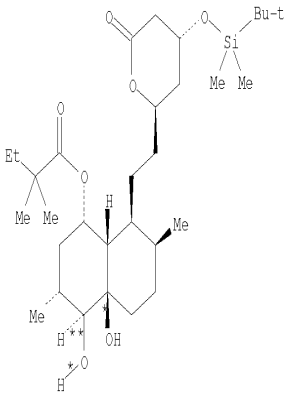
ST aquayamycin total synthesis Hauser reaction pinacol cyclization

IT Cyclization
(pinacol; first total synthesis of aquayamycin)

L7 ANSWER 3 OF 3 CASREACT COPYRIGHT 2009 ACS on STN

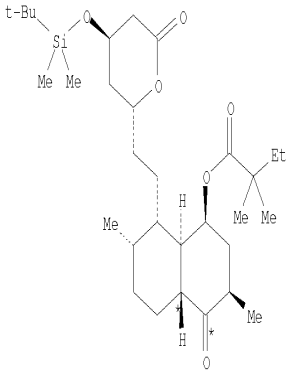
ACCESSION NUMBER: 115:8376 CASREACT <<LOGINID::20090621>>
TITLE: Novel synthesis of mevinolin-related compounds. Large-scale preparation of HMG-CoA reductase inhibitor L-679,336
AUTHOR(S): DeCamp, Ann E.; Mills, Sander G.; Kawaguchi, Alan T.; Desmond, Richard; Reamer, Robert A.; DiMichele, Lisa; Volante, R. P.
CORPORATE SOURCE: Dep. Process Res., Merck Sharp and Dohme Res. Lab., Rahway, NJ, 07065, USA
SOURCE: Journal of Organic Chemistry (1991), 56(11), 3564-71
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

RX(2) OF 3 ...B ===> I



B

(2) →



I

YIELD 87%

RX(2) RCT B 134004-76-5
RGT J 2526-64-9 Ph3PCl2
PRO I 127343-16-2
SOL 141-78-6 AcOEt

AB A novel synthetic route to a mevinolin-related HMG-CoA reductase inhibitor L-679,336 contains as key features a diastereoselective OsO4-catalyzed dihydroxylation reaction and a highly selective, phosphorus-mediated, pinacol-type rearrangement to give ketone I (RR1 = bond). Multinuclear NMR expts. were used to gain a detailed understanding of the pinacol step. The route was used for multikilogram preparation of I (R = R1 = H). Epoxide intermediates underwent Lewis acid-catalyzed rearrangement reactions. Deacylated olefinic substrates II (X = bond, H2) underwent intramol. hydrosilylation reaction.

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FULL ESTIMATED COST                                 147.71     354.81

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     FILE 'CASREACT' ENTERED AT 11:44:39 ON 21 JUN 2009
L2           3 SEA FILE=CASREACT SSS SAM L1 (    13 REACTIONS)
L3         317 SEA FILE=CASREACT SSS FUL L1 (  1474 REACTIONS)
L4          11 SEA FILE=CASREACT SPE=ON  ABB=ON  PLU=ON  L3 AND PINACOL
               D 1-11 IBIB HIT

     FILE 'CASREACT' ENTERED AT 11:52:31 ON 21 JUN 2009
L5             STRUCTURE UPLOADED
               D
L6          49 SEA FILE=CASREACT SSS FUL L5 (   163 REACTIONS)
L7           3 SEA FILE=CASREACT SPE=ON  ABB=ON  PLU=ON  L6 AND PINACOL
               D L7 1-3 IBIB HIT

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COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
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